The Prediction of Bubble Defects in Castings

by

James Andrew Lawrence

Thesis for the Posthumous Award of the Doctor of Philosophy Degree of the University of Greenwich

Material Assembled by K A Pericleous

April 2004

Preface

This document contains a compilation of work carried out by James Andrew Lawrence in the period between 01/11/00 and his untimely death in January 2004, on the subject of the prediction of bubble defects in castings. The compilation contains progress reports and project presentations arranged (roughly) in chronological order. The material was assembled by me - Prof K.A. Pericleous as James' first supervisor - after the event of his death, from various sources but mainly from his desktop PC. This material is not complete, but it is submitted nevertheless as evidence to the examining panel, for the award of a posthumous MPhil/PhD degree.

Although James (an EPSRC-funded student) was due to complete three years of his PhD as a fulltime student in November 2003, he in fact interrupted his FT studies towards the first half of 2003 to pursue his musical career. James remained strongly committed to completing his research, but due to this other opportunity, he altered his registration to PT in September 2003. He used the time away, to concentrate on writing his thesis on a personal laptop he carried with him. Unfortunately we have no access to this laptop and it was considered insensitive under the circumstances to approach his parents for it.

James Andrew Lawrence was transferred from MPhil to PhD in November 2002 with the approval of the Research Degrees Committee, having shown sufficient progress in his research. It is the assessment of his supervisors that, had he not interrupted his fulltime attendance he would be on course for a 3-year completion.

K.A. Pericleous 23.04.04

Abstract

Objective of this research was to develop models that capture the entrainment, breakup and transport of gas bubbles in solidifying TiAl castings. The candidate has reviewed the literature, programmed in FORTRAN code, and validated a number of competing techniques for two phase flow relevant to the filling of moulds. He has developed a hybrid (Donor-acceptor/ Level Set) method, which captures the characteristics of gas bubbles based on the surface tension – fluid inertia balance on the free surface. He has demonstrated the ability of this method to reproduce observed phenomena. The candidate also conducted an experimental campaign in Birmingham University under the supervision of Dr R.A. Harding to provide real casting data for his simulations.

KAP

Edited extract from RD3 MPhil/PhD form: "This research was carried out at the University of Greenwich in conjunction with the University of Birmingham as part of a larger EPSRC-funded project concerned with the development of a casting process route for the production of gamma-TiAl components. Focus of the research was the development of a model of entrained bubbles in the metal casting process. This model comprises the combination of several physical phenomena coupled within the PHYSICA multi-physics framework. The key areas the research has touched on are, surface tension modelling and free-surface modelling using the finite volume technique.

A model has been developed that simulates bubble formation during the filling of castings due to surface entrainment and subsequent motion. Once entrained these bubbles tend to solidify in the casting where the rate of solidification is too fast for escape by buoyancy. This problem is particularly acute in thin blade sections of TiAl, where sufficient superheat cannot be maintained during the casting process. Mould-filling techniques have to be modified accordingly to improve the mechanical integrity of components.

Two phase systems with a sharp, well-defined interface governed by surface tension are required to be modelled. The Level Set Method (LSM) is such a method, used to maintain the position of the interface as it moves through a fixed computational grid. The interface is moved or distorted by the advection equation. In this case two numerical methods are used in differencing: Van-Leer and Donor Acceptor. The Donor Acceptor method is of use when modelling highly dynamic surfaces, such as those encountered during the metal pouring phase in castings, or when fuel sloshes in a fuel tank. This method is best for capturing the entrapment of large bubbles of gas by surface folding. A process directly related to the moving surface. However, the LSM, which allows many surface properties to be calculated, cannot be used in conjunction with the Donor Acceptor method which uses heuristics to sharpen the interface in each compu6tational cell. Once bubbles are formed, their existence and motion are governed by the action of surface tension, therefore the mathematically more rigorous Van-Leer differencing scheme is used in conjunction with the LSM. Bubbles are then tracked using the free-surface method. The tracking limit is determined by the fineness of the mesh used. Sub-

grid bubbles or bubbles that only occupy a small number of cells can no longer be tracked in a continuum Eulerian simulation. Lagrangian particle tracking is then necessary.

The original work in this research can be described as the coupling of the formation of bubbles using the Donor Acceptor method, with the LSM / Van-Leer technique for their subsequent motion and behaviour. This involves:

- Modelling the initial free-surface dynamics with the Donor Acceptor technique.
- Modelling bubble formation using the Donor Acceptor technique.
- Using Results from bubble formation database to "re-start" the simulation with the inclusion of surface tension.
- Tracking bubbles as a free-surface, computing their subsequent break up or coalescence
- Once the bubbles reach a minimum size for a given mesh, continue tracking using the Lagrangian particle tracking technique.

The model was applied to:

- Simple validation experiments to test the correctness of the coding
- Sloshing/collapsing column experiments to evaluate bubble formation
- Simple geometry situations where the combined model is used with Bubble Formation / Tracking / Surface Tension
- Model the filling of the flat plate experimental setup

Future work *(not completed...)*

- Develop criteria for switching between the Eulerian (free surface) and Lagrangian (particle tracking) scheme
- Compare with Experimental Data obtained at the University of Birmingham
- Run 3D Cases representing real geometries with HT and solidification
- Model the counter-gravity filling process"

Contents List

Document # 1
Date: 04/12/00
Name: James Lawrence (University of Greenwich)
Title: Monthly PhD progress report (Nov-Dec 00)

Introduction

The purpose of this report is to provide information on a monthly basis as to what I have been doing and what progress I have made. I have left out the period running from Oct-Nov 00, as this was an adjustment period. It is planned to produce a report at the beginning of each month.

Projects

The following projects have been worked on during the period Nov-Dec 00.

1. 2D modelling of the melting of pure gallium in a rectangular cavity: This involved using PHYSICA and FEMGV to produce the model. This required creation of the geometry and the INFORM file. The model is a test case produced by Peter M-Y Chow in his PhD thesis-Control volume unstructured mesh procedure for convection-diffusion solidification processes (1993).

   To date the following has been achieved:

   i) Geometry has successfully been created using FEMGV.
   ii) The INFORM has been written for the model.
   iii) The case has been run.
   iv) As yet no fully converged solution has been met.

2. PHOENICS workshop Nov 2000: This was a tutorial case that involved the 2D modelling of flow in a duct with a blockage and was created by K.Pericleous. This required the use of PHOENICS to create the geometry and specify boundary conditions.

   To date the following has been achieved:

   i) Geometry has been successfully created.
   ii) Boundary conditions have been specified.
   iii) The case has been run.
   iv) A solution has been reached.

v) No validation of the case has taken place as yet.

3. FORTRAN programming: A program is being created by myself to solve a 1D steady state diffusion problem allowing specification of the problem and solution.

4. Reading: I have been reading the suggested material in the areas of CFD, Casting, FORTRAN programming and general fluid mechanics.

5. General: I have been doing tutorials in PHOENICS and FEMGV/PHYSICA.

Proposed plan of action

Between now and Christmas I plan to do the following:

1. Reach a converged solution for the 2D-gallium model.
2. Validate the results for the PHOENICS tutorial.
3. Create a FORTRAN program for the 1D diffusion problem, and extend the program to 2D and possibly 3D.
4. Carry on reading as much relevant material as possible.

If anyone has any suggestions or comments, please do not hesitate to get in contact:

j.a.lawrence@gre.ac.uk

Document # 2
Date: 23/01/01
Name: James Lawrence (University of Greenwich)
Title: Monthly PhD progress report (Dec 00-Jan 01)

Projects

The following projects have been worked on during the period Dec 00-Jan 01.

3. 2D modelling of the melting of pure gallium in a rectangular cavity: This involved using PHYSICA and FEMGV to produce the model. This required creation of the geometry and the INFORM file. The model is a test case produced by Peter M-Y Chow in his PhD thesis-Control volume unstructured mesh procedure for convection-diffusion solidification processes (1993).

   To date the following has been achieved:

   v) Geometry has successfully been created using FEMGV.
   vi) The INFORM has been written for the model.
   vii) The case has been run.
   viii) A successful converged solution has been reached.
   ix) An animation has been created available at www.gre.ac.uk/~lj59/
   x) A full report has been compiled and is also available.

4. Mathematics tutorials concerning the fundamental governing equations. These tutorials have been taken by Koulis Pericleous and have covered the following topics.

   vi) PDE to FDE for transport equations of a conserved variable.
   vii) Development of the Navier – Stokes equations.
   viii) Discussions have also taken place as to the nature of the equations relating to the 2D model created above.

3. Reading: I have been reading the suggested material in the areas of CFD, Casting, FORTRAN programming and general fluid mechanics as before. I have also been reading papers concerning numerical modelling of phenomena relating to casting, such as buoyancy driven flows, free surface flows, Solidification and stress deformation.

Proposed plan of action

I plan to carry on with the following for the next month or so:

5. Read and understand papers relating to free surface flows.

6. Create a numerical model of a collapsing liquid column using PHYSICA (free surface flow model).
3. Attempt to simulate the filling of some casting test pieces.

If anyone has any suggestions or comments, please do not hesitate to get in contact:
j.a.lawrence@gre.ac.uk

Document # 3

Laminar Natural-convection and heat transfer for the melting of pure Gallium in a two-dimensional rectangular cavity

James Lawrence
PhD Monthly Progress Report, January 2001-02-06
Supervisors: KA Pericleous, V Bojarevics, RA Harding #
University of Greenwich: CMS
University of Birmingham: IRC for Advanced Materials

Abstract - The following reports on the computational method used to solve buoyancy driven laminar flow and heat transfer for the melting of pure Gallium in a two-dimensional enclosed rectangular cavity with differentially heated vertical walls. The results are presented in graphical form and compared with benchmark numerical and experimental cases. Comments are made as to the ability of the PHYSICA code in handling this type of flow.
The model was built using FEMGEN v.6.1-02 according to an experimental specification established by Gau and Viskanta (See Chow 1993). An under-relaxation value of 0.8 was required for heat transfer and pressure correction and a false time step 0.1 was required for the two momentum equations. The melt front was plotted by using a 0.5 value for the liquid fraction.
Results from the current study compared well with the benchmark cases, thus proving the suitability of PHYSICA for solving flows of this nature.

1 Introduction

Buoyancy driven flows have many practical applications such as double-glazing, room ventilation, solar energy collection and casting. This type of flow has been studied both experimentally by Gau and Viskanta and numerically by Brent et al as detailed by Chow (1993) and references within, thus enabling good comparison of the results. The geometry and boundary conditions used were the same used for both the numerical and experimental cases (Chow 1993). Much work has been done in this area (Markatos & Pericleous 1984) and the problem considered provides a good means of testing different numerical techniques for solving buoyancy driven flows.

2 Problem Description

The problem is shown diagrammatically in Fig.1. The hot wall is assumed to be at a constant 311.0K and the cold wall at a constant 301.3K. The Gallium is assumed to be solid at 0 seconds at a temperature of 301.3K, which is below the melting point of 302.78K. The top and bottom edges are assumed to be insulated. This is a transient problem where a convection diffusion phase change occurs.

Heat transfer through the isothermal hot wall causes the initial phase change from solid to liquid and further heat transfer causes a density variation in the liquid. This leads to buoyancy-driven recirculation. The flow is assumed to be laminar (Ra $\leq 10^6$ see apendix 1) and walls assume a non-slip boundary condition with velocity components u=v=0 ms^{-1}. The x and y dimensions are 8.89cm and 6.35cm respectively. For the INFORM file detailing input of the boundary conditions see appendix 2.

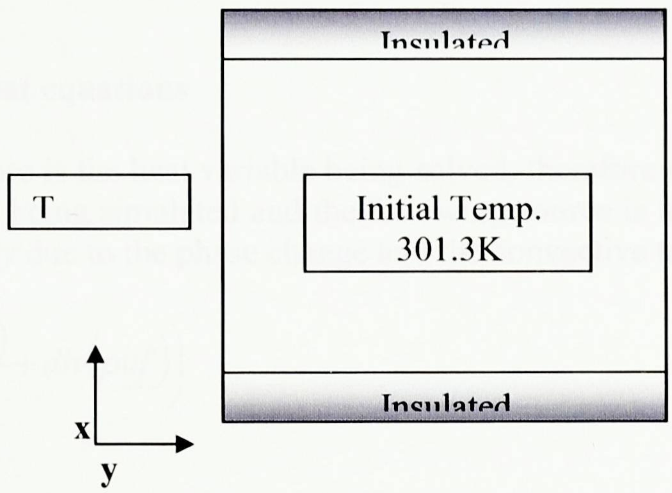


Fig.1. Boundary conditions used - Gau and Viskanta (see Chow 1993)

3 Mathematical Model

In the PHYSICA code the general conservation equation is expressed as

$$\frac{\partial(Ct\phi)}{\partial t} + div(Ccu\phi) = div(\Gamma_\phi grad(\phi)) + S\phi \tag{1}$$

where ϕ is the conserved quantity, C_t is the coefficient of the transient term, C_c is the coefficient of the convection term and Γ is the diffusion term.

3.1 Momentum equations

The gravity vector is set in the negative y direction, which means a buoyancy source is added. In this case the buoyancy source takes the following form in the momentum equations:

$$\rho_{ref}\beta(T_{ref} - T)g_i \tag{2}$$

where ρ_{ref} is the reference density, T_{ref} is the reference temperature, β is the coefficient of thermal expansion and T is the temperature.
A Darcy type source is also added in this case to account for the effects of flow resistance in the partially *mushy zone*.

$$-u_i \frac{(1-f)^2}{f^3} K \qquad (3)$$

where f is the liquid fraction and K is the permeability coefficient.

3.2 Heat equations

Temperature is the heat variable being solved, therefore no default source terms are used. Melting is being simulated and the following source is used to account for the change in heat energy due to the phase change and the convective transfer of the liquid.

$$-L\left(\frac{\partial(\rho f)}{\partial t} + div(\rho \underline{u} f)\right) \qquad (4)$$

In this case L is the latent heat and f is the liquid fraction.

4 Results and Discussion

Results from the present simulation are presented in graphical form at the approximate times of 1min, 2mins, 3mins, 6mins, 8mins, 10mins, 12mins, 15mins, 17mins and 19mins showing the progress of the melt front. This was achieved by plotting a 0.5 value for the liquid fraction at intervals of 50secs. Comparisons are made with both experimental and numerical results to assess the accuracy of the PHYSICA code in solving the problem. Velocity vectors and temperature contours at 3mins and 19mins are also presented and a comparison is made between the work by Chow and the current study.
It can be seen from Fig.2 that the PHYSICA code produces results that correlate well with the benchmark results detailed in Chow (1993) when considering the general development of the melt front. The results show the initial heat conduction melting of the Gallium at approximately 1 and 2 minutes, demonstrated by a melt front that is approximately perpendicular to the x-axis. At 6 minutes the characteristic profile of the buoyancy driven flow starts to show. As the liquid Gallium heats up a decrease in density occurs causing hot liquid to rise and transfer heat to the adjacent solid Gallium, thus cooling, increasing in density and sinking, setting up a convection current (Incropera & Dewitt 1996), producing the familiar profile of the melt front. As time increases the profile becomes more prominent and at approximately 19 minutes the convective flow is well established. This is shown in both the experimental and numerical benchmark cases.

In the current study the results seem to be dominated by convection showing a more pronounced melt front profile at increased time steps. This can be demonstrated more clearly by inspecting the temperature contours for the current study and Chow (1993) (Figs.3 &5). At three minutes the isotherms are near vertical indicating that the main heat transfer mechanism is conduction. As the time steps increase the isotherms depart from the vertical and this shows that the main mechanism for heat transfer is convection. When the results from the current study are compared with the benchmark results it can be seen that at 19 minutes the isotherms have detracted from the vertical axis considerably more than shown by Chow (1993). This can also be seen in the resultant velocity vector plots (Figs. 3 &5). As the isotherms become less vertical temperature stratification occurs causing the central region of the convective flow to be closer to the centre of the cavity.and a difference in this centre position can be noticed between Figs. 3 & 5 (19 mins). This convective flow is driven by the temperature gradient across the cavity $\partial T / \partial y$ and as this gradient increases so does the contribution of convection.

The same simulation was also run for different grids (detailed in section4.1) and it was found that if a coarser grid was used (22x12) the isotherms were less obscured from the vertical at increased time-steps thus showing that convection was having a reduced effect on heat transfer (Fig.4). The grid resolution could therefore explain the differences in results from the current study using a 42x 32 grid and the benchmark results

4.1 Computational Requirements

A uniform mesh size of 42x32 (1344 cells) was used as used by Chow(1993). This was adequate as no slip conditions were applied to all walls; therefore near wall regions did not require any further grid resolution. A 100 time-step run took 21 minutes CPU time on a Pentium III 733MHz PC. The solution seemed to converge without difficulty. The main variables of interest were u-velocity (u), v-velocity (v), temperature (TN) and liquid (LF) fraction. Typical values of the residuals in the first and last time step are shown in Table.1.

Variable	Time-Step	Residual
u	1	3.998E-13
v	1	8.582E-12
TN	1	2.685E+01
LF	1	1.013E-01
u	final	1.771E-06
v	final	1.568E-06
TN	final	9.894E-04
LF	final	1.620E-04

Table.1. Typical residual values (42x32 grid)

Further runs were carried out with a 22x12 grid (264 cells) and a 72x62 grid (4464 cells). A 100 time-step run with the 22x12 grid took 1.2 minutes on the same CPU as used above and seemed to produce results similar to the 42x32 grid, but seemed to be less affected by convection in the latter stages of the melting process. A 100 time-step run with the 72x62 had considerable problems with convergence.

5 Conclusion

The PHYSICA code gives results similar to existing numerical and experimental data thus proving its capability in solving buoyancy driven flows with phase change. Grid resolution did appear to have an effect on the results. As a first - time user of PHYSICA the problem seemed relatively easy to solve with only a few minor problems causing a delay in obtaining a final solution. These problems were mainly due to user error and unfamiliarity with the code. There were no obvious flaws in the code related to solving this type of flow. Care has to be taken regarding default settings and every effort should be made to that correct settings are enabled.

5.1 Future Work

In the foreseeable future work is to be carried out in modelling free surface movement with heat transfer and phase change under the action of gravity using the PHYSICA code. This will only be done in a two-dimensional square cavity. In order to do this the free surface flow will be modelled first and the heat transfer and solidification phenomena will be subsequently added.
Free Surface problems are encountered in the filling and emptying of containers and with the heat transfer and solidification the problem is particularly applicable to the design of moulds for the casting of metals.
It is also planned to relate the free surface problem to the filling of some laboratory test pieces. This is then to be validated at the IRC for advanced materials.

6 References

1. Chow, "Control Volume Unstructured Mesh procedure for Convection – Diffusion Solidification Process", 1995, PhD thesis, University of Greenwich.

2. N. C. Markatos & K. A. Pericleous, International Journal of Heat and Mass Transfer vol. 27, No. 5, pp. 755-772, "Laminar and turbulent natural convection in an enclosed cavity", 1984,
Pergamon Press.

3. Centre for Numerical Modelling and Process Analysis, School of Computing and Mathematical Sciences, The University of Greenwich, London, UK, "PHYSICA Version 2.11 Users Guide", 1999, the University of Greenwich.

4. H. K. Versteeg & W. Malalasekera, "An introduction to Computational Fluid Dynamics the Finite Volume Method", 1995, Longman Group Ltd.

5. F. P. Incropera & D. P. Dewitt, "Fundamentals of Heat and Mass Transfer", 1996, Wiley and Sons Inc.

6. J. F. Douglas, J. M. Gasiorek & J. A. Swaffield, "Fluid Mechanics", 1998, Longman Group.

7. J. Campbell, "Castings", 1991, Butterworth-Heinmann Ltd

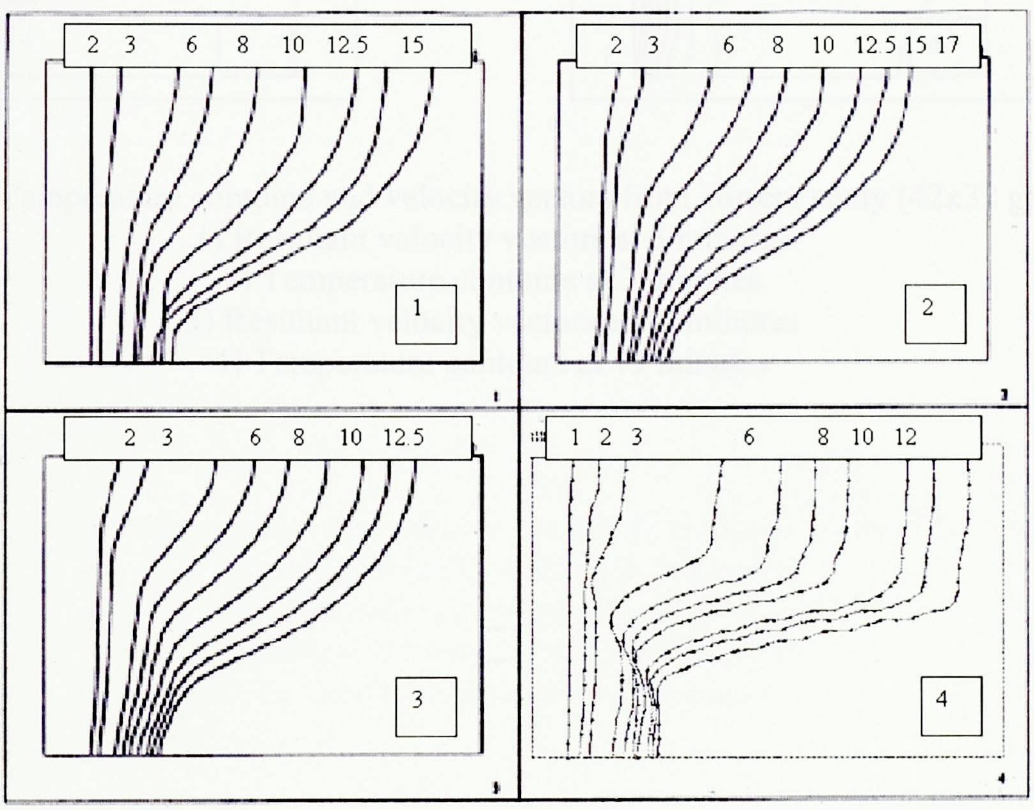


Fig.2. Gallium melt fronts plotted in minutes
1) Experimental results of Gau and Viskanta – Taken from Chow (1993)
2) Numerical results of Brent et al – Taken from Chow (1993)
3) Numerical results of Chow (1993)
4) Numerical results from current study

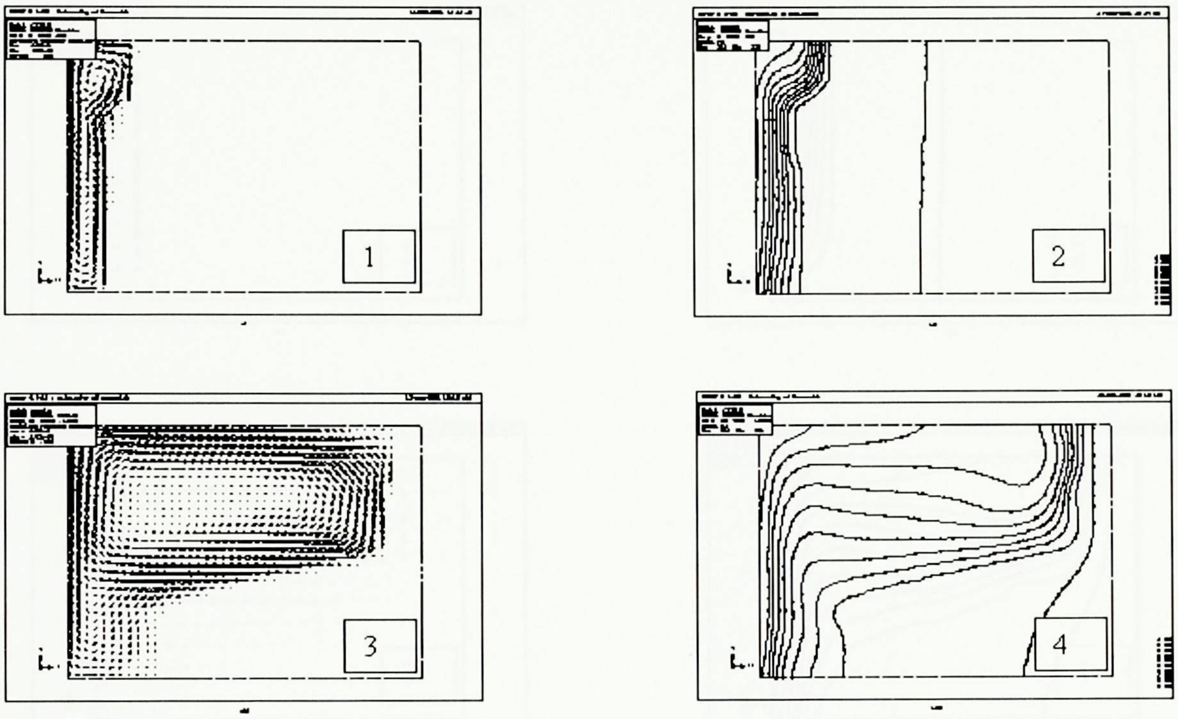


Fig.3. Temperature contours and velocity vectors from current study (42x32 grid)
1) Resultant velocity vectors at 3 minutes
2) Temperature contours at 3 minutes
3) Resultant velocity vectors at 19 minutes
4) Temperature contours at 19 minutes

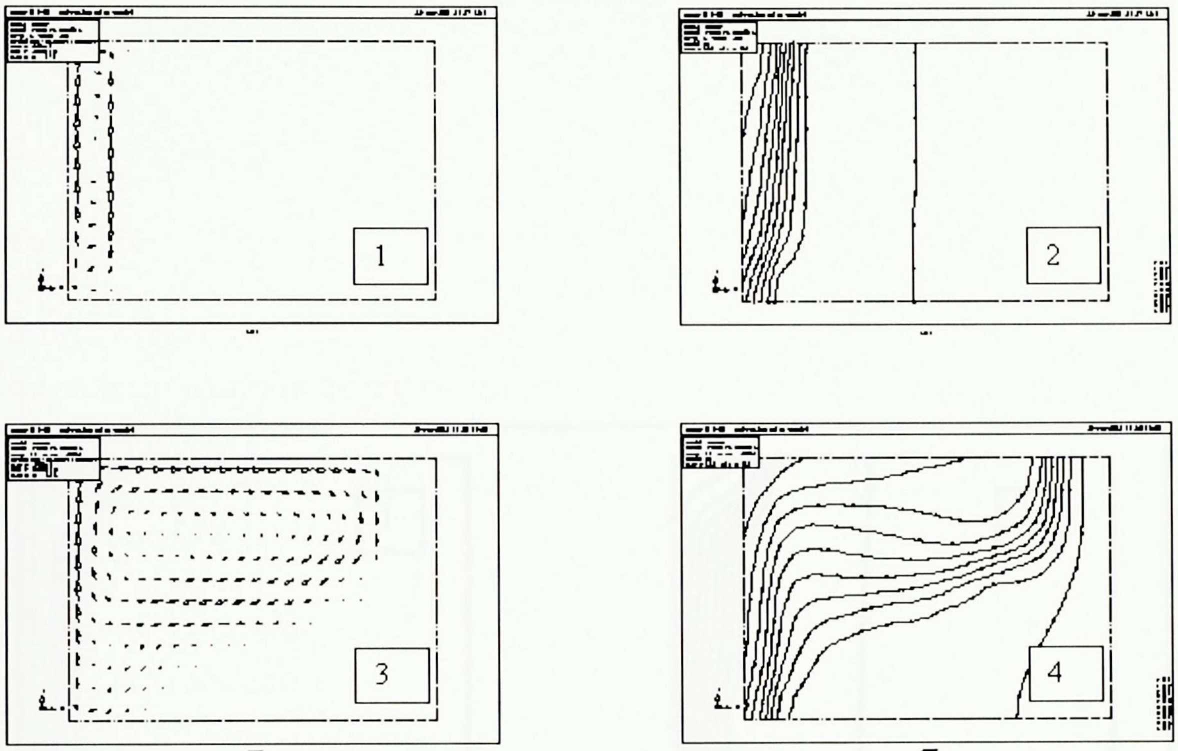


Fig.4. Temperature contours and velocity vectors from current study (22x12 grid)
1) Resultant velocity vectors at 3 minutes
2) Temperature contours at 3 minutes
3) Resultant velocity vectors at 19 minutes
4) Temperature contours at 19 minutes

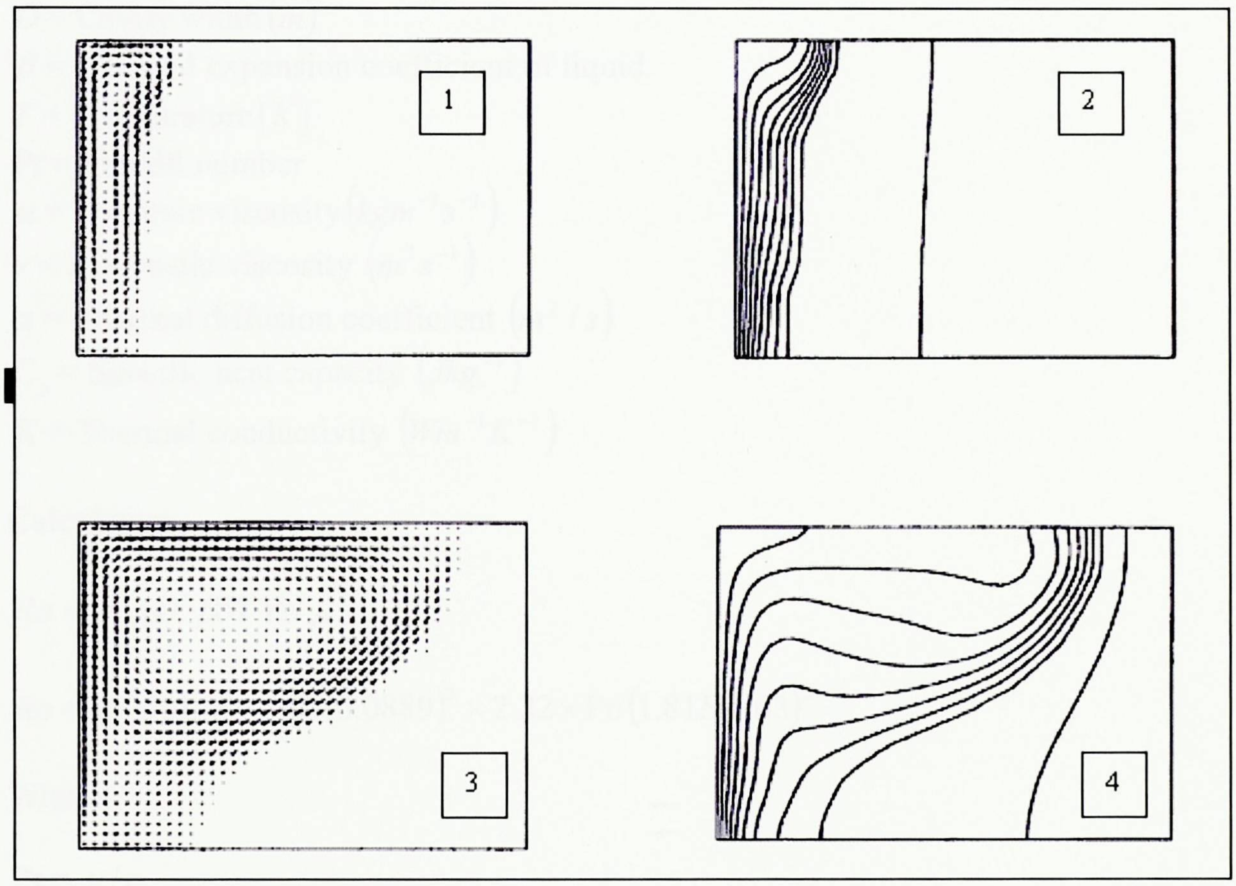


Fig.5. Temperature contours and velocity vectors (Chow 1993)
1) Resultant Velocity vectors at 3 minutes
2) Resultant Temperature contours at 3 minutes
3) Velocity vectors at 19 minutes
4) Temperature contours at 19 minutes

Appendix 1 Rayleigh number determination

$$Ra = \rho^2 g D^3 \beta \delta T \, \mathrm{Pr} / \mu^2$$

Nomenclature

ρ = Density $\left(kgm^{-3}\right)$
g = Gravitational acceleration $\left(ms^{-2}\right)$
D = Cavity width (m)
β = Thermal expansion coefficient of liquid
T = Temperature (K)
Pr = Prandtl number
μ = Dynamic viscosity $\left(kgm^{-1}s^{-1}\right)$
ν = Kinematic viscosity $\left(m^2 s^{-1}\right)$
α = Thermal diffusion coefficient $\left(m^2/s\right)$
C_p = Specific heat capacity $\left(Jkg^{-1}\right)$
K = Thermal conductivity $\left(Wm^{-1}K^{-1}\right)$

Calculation

$$Ra = \rho^2 g D^3 \beta \delta T \, \mathrm{Pr} / \mu^2$$

$$Ra = (6093)^2 \times 9.81 \times (0.0889)^3 \times 2.22 \times \mathrm{Pr} / (1.81E-03)^2$$

Where,

$\mathrm{Pr} = \nu / \alpha$
$\alpha = K / C_p$
$\mathrm{Pr} = 0.022$

Therefore,

$$Ra = 1092348.5 \langle 10^6$$

Therefore, flow is laminar

Appendix 2 INFORM file

```
# ****2-D Melting of Gallium By J. Lawrence Jan 2001*****

GEOMETRY_MODULE
  FILENAME  caseG
  GRAVITY_Y  -9.81
END

GENERIC_MODULE
# STEADY_STATE_RUN
MAX_SWEEPS 1000
  TRANSIENT_RUN
    DELTA_T
      FOR_ALL_TIME_STEPS  5
    END
    TOTAL_TIME_STEPS 240
  END
END

MONITOR_MODULE
  OUTPUT_INTERVAL  100
  SPOT_VALUE  16
END

MATERIAL_PROPERTY_MODULE
  DENSITY
    MATERIAL 1 CONSTANT 6093.0
  END

  THERMAL_CONDUCTIVITY
    MATERIAL 1 CONSTANT 32.0
  END

  SPECIFIC_HEAT
    MATERIAL 1 CONSTANT 381.5
  END
  LATENT_HEAT
```

```
    MATERIAL 1 CONSTANT 80160.0
  END

   LIQUIDUS_TEMPERATURE
    MATERIAL 1 CONSTANT 302.78
   END

   SOLIDUS_TEMPERATURE
    MATERIAL 1 CONSTANT 302.78
   END

  THERMAL_EXPANSION_COEFFICIENT
    MATERIAL 1 CONSTANT 1.2E-04
  END

  VISCOSITY
    MATERIAL 1 CONSTANT 2.97E-7 1.81E-03
  END
END
HEAT_TRANSFER_MODULE
HEAT_UNDER_RELAXATION 0.8
# HEAT_FALSE_TIMESTEP 1E+3 0.8
  SOLVE_TEMPERATURE
    INITIAL_VALUES ALL 302
    BOUNDARY_CONDITIONS
      PATCH 1 FIXED_VALUE VALUE 311.0
      PATCH 2 FIXED_VALUE VALUE 301.3
    END
  END
END
SOLIDIFICATION_MODULE
  FRACTION_LIQUID_FUNCTION
    MATERIAL 1 LINEAR_FUNCTION
  END
END

FLUID_FLOW_MODULE
PRESSURE_UNDER_RELAXATION 0.8
MOMENTUM_FALSE_TIMESTEP  0.1

  BUOYANCY
    BOUSSINESQ_APPROXIMATION  ON
    REFERENCE_DENSITY  6095.0
    REFERENCE_TEMPERATURE 302.78
  END
  SOLVE_U-MOMENTUM
```

```
    INITIAL_VALUES ALL 0.0
    BOUNDARY_CONDITIONS
      PATCH 1 WALL COEFF 1.0 VALUE 0.0
      PATCH 2 WALL COEFF 1.0 VALUE 0.0
      PATCH 3 WALL COEFF 1.0 VALUE 0.0
      PATCH 4 WALL COEFF 1.0 VALUE 0.0
    END
  END

  SOLVE_V-MOMENTUM
    INITIAL_VALUES ALL 0.0
    BOUNDARY_CONDITIONS
      PATCH 1 WALL COEFF 1.0 VALUE 0.0
      PATCH 2 WALL COEFF 1.0 VALUE 0.0
      PATCH 3 WALL COEFF 1.0 VALUE 0.0
      PATCH 4 WALL COEFF 1.0 VALUE 0.0
    END
  END

  SOLVE_PRESSURE
    INITIAL_VALUES ALL 0.0
  END

  PRESSURE_REFERENCE_POINT 16
END

POST-PROCESSING_FORMAT
  FEMGV_FORMAT
    SET_FEMVIEW_WRITE 10
  END
END

STOP
```

Document # 4
Date: 02/05/01
Name: James Lawrence (University of Greenwich)
Title: Monthly PhD progress report (Mar 01-May 01)

Projects

The following projects have been worked on during the period Mar 01-May 01.

5. Fortran programming: Developing codes to solve

   i) 1D Diffusion.
   ii) 1D Convection diffusion.
   iii) 2D Convection Diffusion.
   iv) 3D Diffusion.

   The above codes have been written and implemented using the Tri-diagonal matrix algorithm as a solver ("An introduction to Computational Fluid Dynamics The Finite Volume Method", HK Versteeg & W Malalasekera, Longman Group 1995).
   Work has also been carried out to try and implement the SIMPLE algorithm for coupled pressure-velocity problems where no initial field is known ("An introduction to Computational Fluid Dynamics The Finite Volume Method", HK Versteeg & W Malalasekera, Longman Group 1995). This was understood, but not fully implemented.

2. Free surface modelling: Free surface models have been developed in 2D to represent simple filling problems. An imaginary geometry was created and an INFORM was written as usual and is attached to this report along with the geometry, mesh and boundary conditions. The problem was solved twice using two different convection schemes (Van Leer & Donor Acceptor method see INFORM). The models worked and animations are available.

3. Three dimensional mesh generation: After receiving a set of engineering drawings from Dr. Harding representing top and bottom filled mould designs, an effort has been made to produce a 3D mesh in order to model the filling process. This first involves working out how to create the geometry in a way that lends itself to good meshing practices. This has been done, but as ever is always subject to further refinement. At this present moment in time I am attempting to create a mesh for the geometry, which is a lengthy iterative process. However, when some results come from this model I will let everyone know.

6. Reading:
   i) **"A Computational Model for Defect Prediction in Shape Castings Based on the Interaction of Free Surface Flow, Heat Transfer, and Solidification Phenomena"**, S.Bounds, G.Moran, K.Pericleous, M.Cross,

and T.N.Croft, Metallurgical and Materials Transactions B Volume 31B, June 2000.

ii) **"The Running and Gating of Light Alloys"**, J.Runyoro and J.Campbell, The Foundryman, April 1992.

iii) **"Three-dimensional Free Surface Modelling in an Unstructured Mesh Environment For Metal Processing Applications"**, K.A.Pericleous, G.J.Moran, S.M.Bounds, P.Chow, M.Cross, Applied Mathematical Modelling 22, 1998.

Proposed plan of action

I plan to carry on with the following for the next month or so:

1. Simulate the filling of the mould geometry from Birmingham.
2. Establish whether surface turbulence leading to bubble formation is observed in both top and bottom filling as instructed by Dr. Harding.
3. Repeat the above with appropriate heat models.
4. Repeat the above with both high and low superheat.

If anyone has any suggestions or comments, please do not hesitate to get in contact: j.a.lawrence@gre.ac.uk

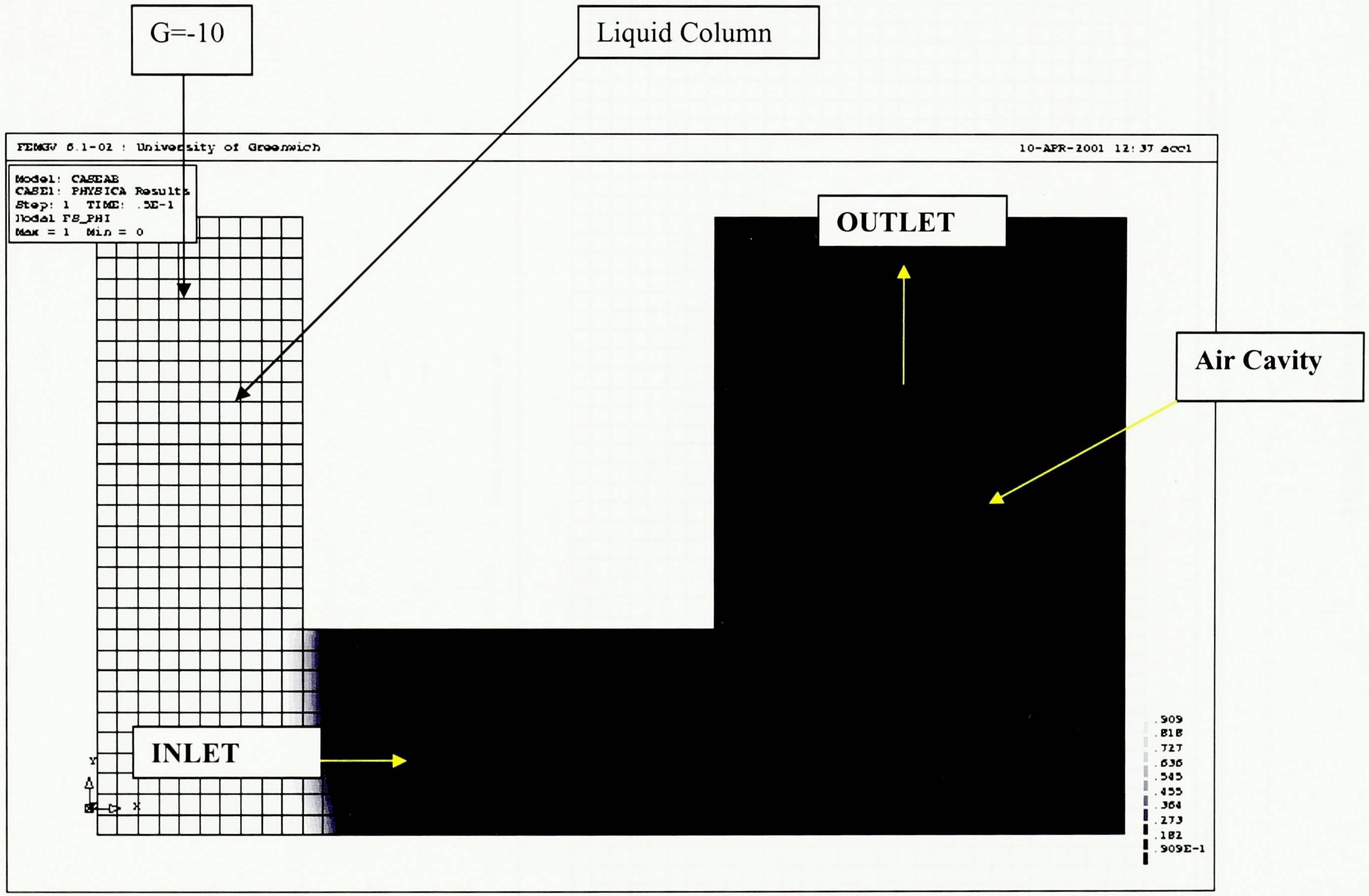
INFORM File.
James Lawrence 02/05/01

```
#  Free surface mold filling
#  James Lawrence
#  University of Greenwich
#
GEOMETRY_MODULE
  FILENAME caseab
  GRAVITY_Y -10.0
END

GENERIC_MODULE
  TRANSIENT_RUN
    DELTA_T
      USER_DELTA_T
      FOR_ALL_TIME_STEPS 0.005
    END
    END_TIME 2.00
    SAVE_AT_EVERY_TIME_STEP -1
  END
  MAX_SWEEPS 30
END

MONITOR_MODULE
  OUTPUT_INTERVAL 10
  FRACTION_DIGITS 5
  BLOCK_FORMAT ON
END

POST-PROCESSING_FORMAT
  FEMGV_FORMAT
    SET_FEMVIEW_WRITE 10
  END
END
```

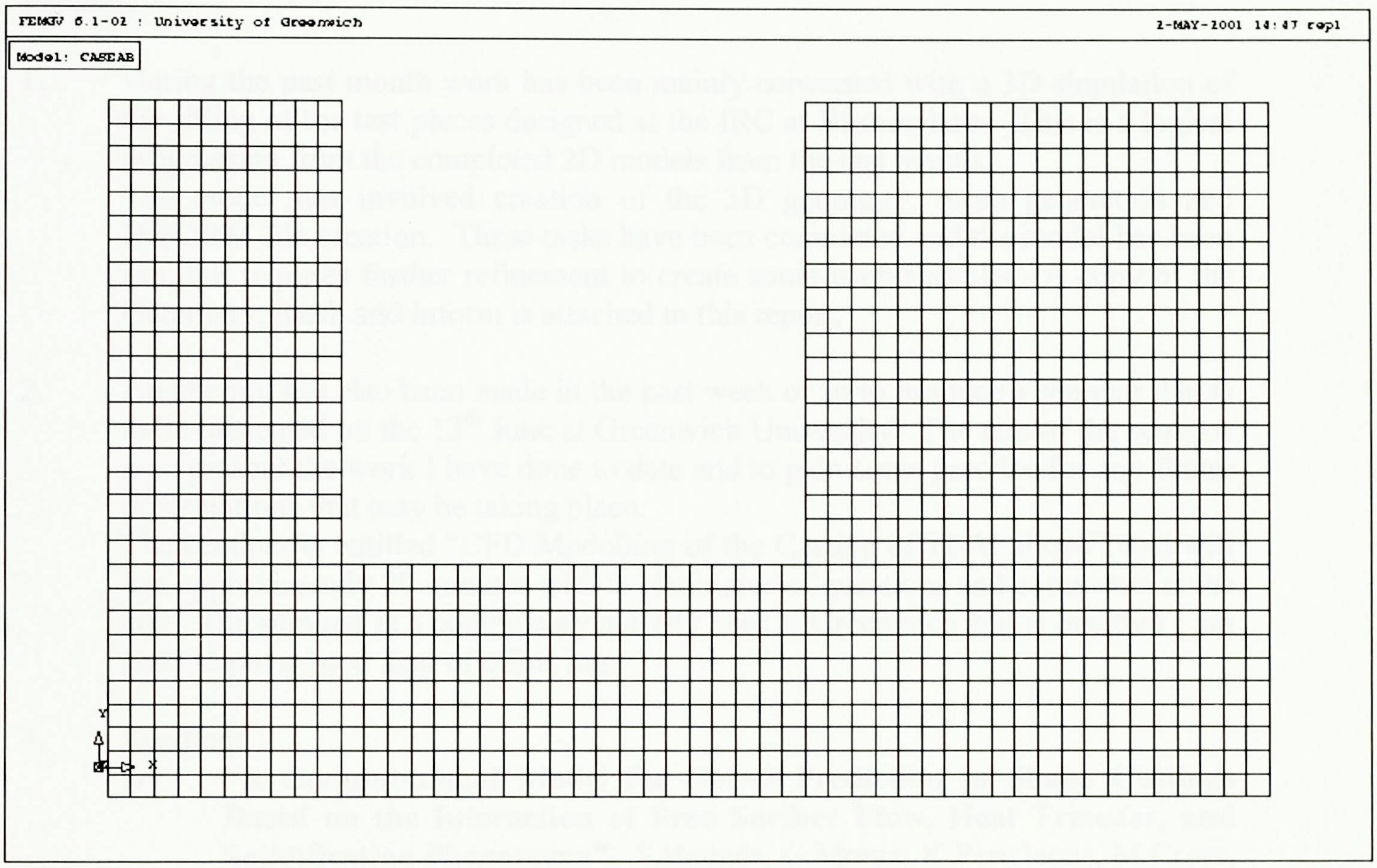
```
FREE_SURFACE_MODULE
  EXPLICIT_FACTOR 1.0
#  CONVECTION_METHOD  DONOR_ACCEPTOR
  CONVECTION_METHOD VAN_LEER
  EXPLICIT_SOLUTION_STAGE START_OF_TIME_STEP
  GALA ON
  SOLVE_FREESURF
    INITIAL_VALUES USER_ROUTINE perpatch 2 0.0 1.0
  END
#  BOUNDARY_CONDITIONS
#    PATCH 1 FIXED_VALUE VALUE 1.0
#  END
END

MATERIAL_PROPERTY_MODULE
  DENSITY
    MATERIAL 1 USER_ROUTINE FS_PROP 2 1000.0 1.0
    SAVE_PROPERTY END_OF_RUN
  END
  VISCOSITY
    MATERIAL 1 CONSTANT 0.0 1.0E-08
  END
END

FLUID_FLOW_MODULE
  BUOYANCY
    REFERENCE_DENSITY 1.00
  END
  SOLVE_U-MOMENTUM
    INITIAL_VALUES ALL 0.0
#    BOUNDARY_CONDITIONS
#    PATCH 3 WALL COEFF 1.0 VALUE 0.0
  END
  SOLVE_V-MOMENTUM
    INITIAL_VALUES ALL 0.0
#    BOUNDARY_CONDITIONS
#    PATCH 3 WALL COEFF 1.0 VALUE 0.0
  END
  SOLVE_W-MOMENTUM
    INITIAL_VALUES ALL 0.0
  END
  SOLVE_PRESSURE
    INITIAL_VALUES ALL 0.0
    BOUNDARY_CONDITIONS
      PATCH 1 FIXED_VALUE VALUE 0.0
```

```
      PATCH 2 FIXED_VALUE VALUE 0.0
    END
  END
END

STOP
```

Boundary Conditions at T=0s
James Lawrence 02/05/01



2D Geometry and Mesh for free Surface Filling problem
James Lawrence 02/05/01



2D Geometry and Mesh

Document # 5
Date: 29/05/01
Name: James Lawrence (University of Greenwich)
Title: Monthly PhD progress report (May 01-June 01)

Projects

1. During the past month work has been mainly concerned with a 3D simulation of the filling of the test pieces designed at the IRC at Birmingham. This is a logical progression from the completed 2D models from the last month.
   The model has involved creation of the 3D geometry, mesh generation and INFORM file creation. These tasks have been completed and the model has been run, but requires further refinement to create some useful results. A copy of the Geometry, mesh and inform is attached to this report.

2. An attempt has also been made in the past week or so to produce a seminar that is to be presented on the 13th June at Greenwich University. The aim of the seminar is to present the work I have done to date and to gain some practice for any future presentations that may be taking place.
   The seminar is entitled "CFD Modelling of the Casting of Ti-Al alloys", and will last approximately 20 minutes with 5-10minutes of questions and comments at the end. The seminar is a compulsory activity here at Greenwich and is one that I am keen to put a good deal of effort into.

3. Reading:
   iv) **"A Computational Model for Defect Prediction in Shape Castings Based on the Interaction of Free Surface Flow, Heat Transfer, and Solidification Phenomena"**, S.Bounds, G.Moran, K.Pericleous, M.Cross, and T.N.Croft, Metallurgical and Materials Transactions B Volume 31B, June 2000.
   v) **"The Running and Gating of Light Alloys"**, J.Runyoro and J.Campbell, The Foundryman, April 1992.
   vi) **"Three-dimensional Free Surface Modelling in an Unstructured Mesh Environment For Metal Processing Applications",** K.A.Pericleous, G.J.Moran, S.M.Bounds, P.Chow, M.Cross, Applied Mathematical Modelling 22, 1998.

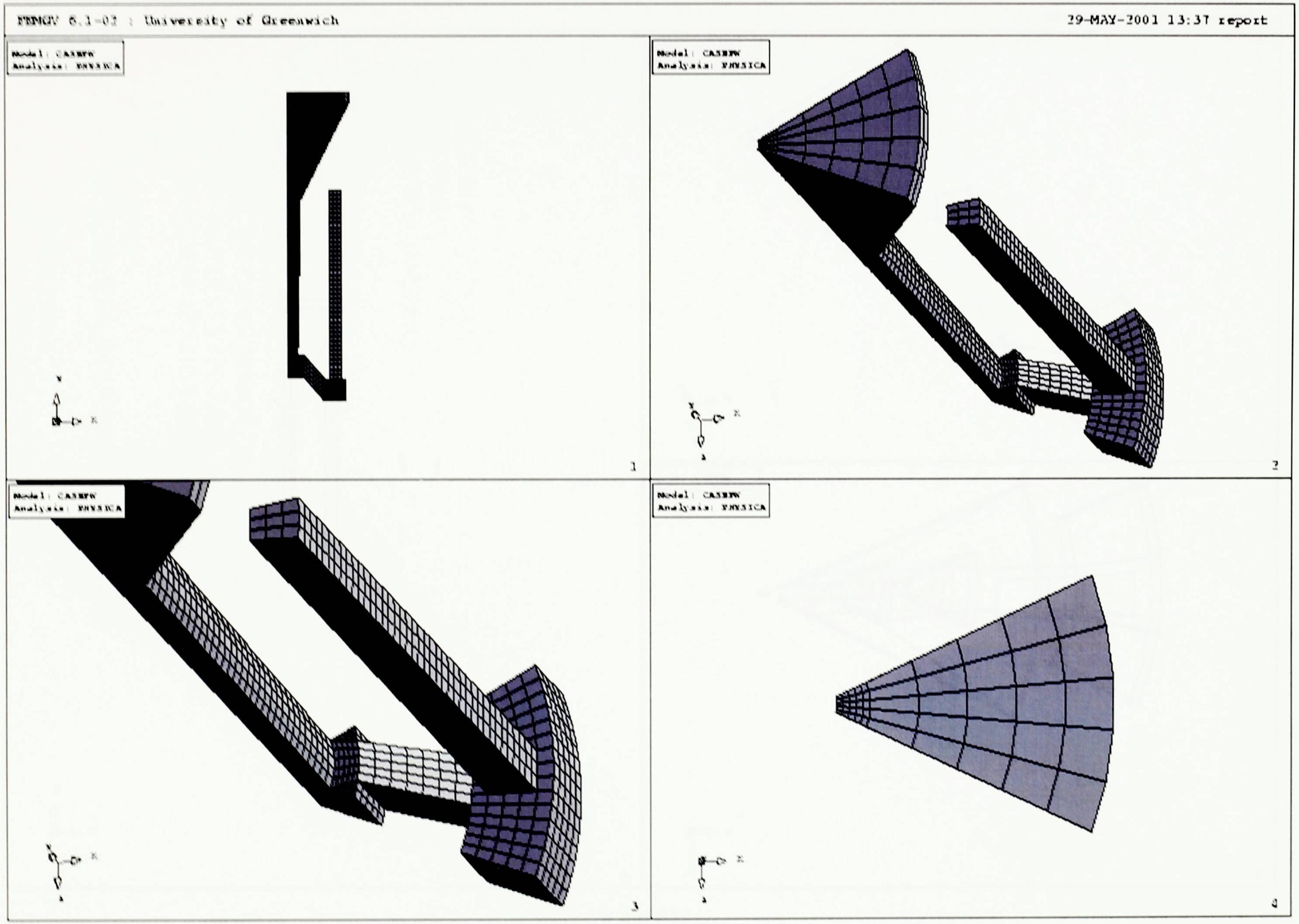
Proposed plan of action

I plan to carry on with the following for the next month or so, which is basically the same as last month and will let everyone know if there are any changes or results:

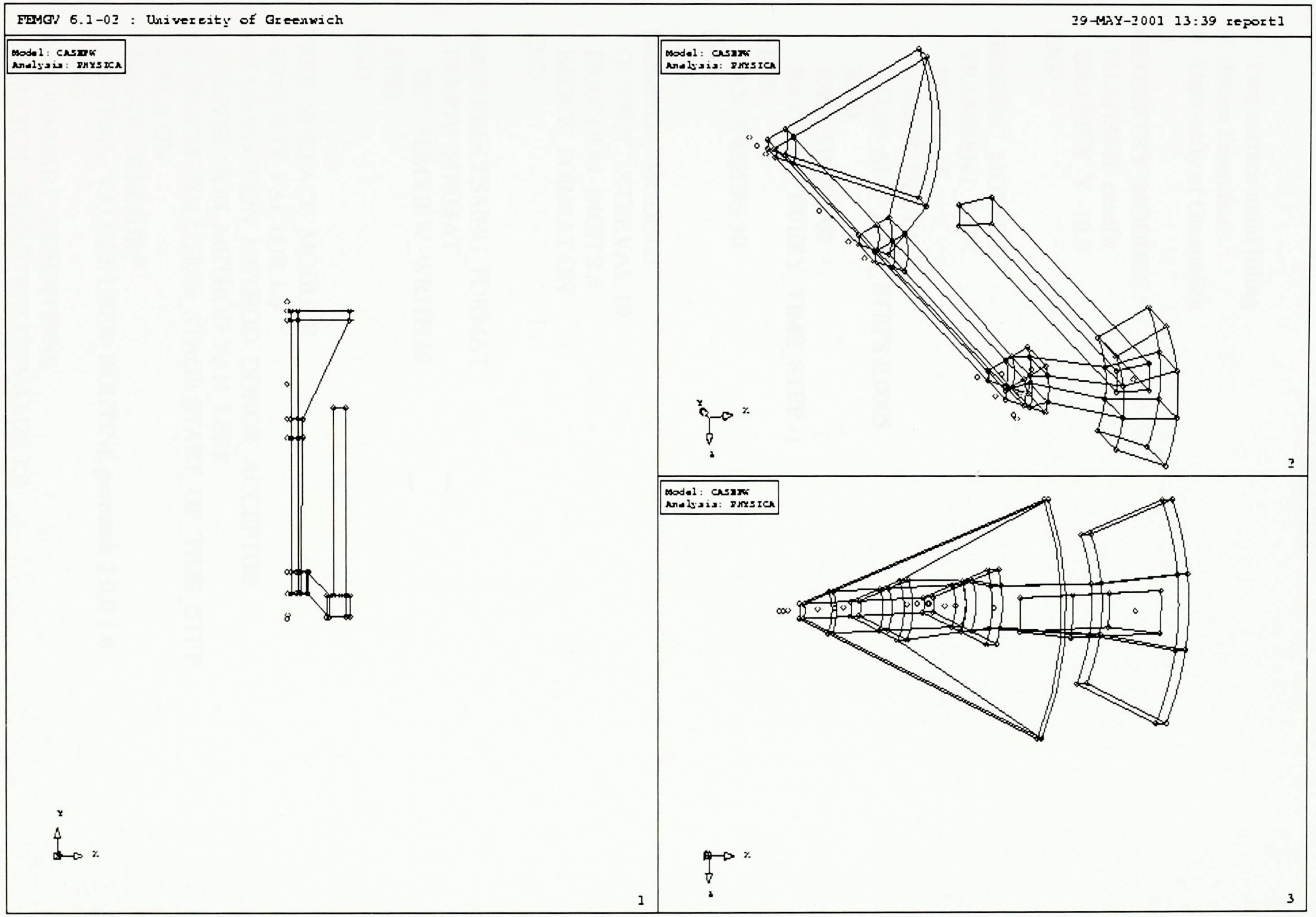
5. Simulate the filling of the mould geometry from Birmingham.
6. Establish whether surface turbulence leading to bubble formation is observed in both top and bottom filling as instructed by Dr. Harding.
7. Repeat the above with appropriate heat models.

8. Repeat the above with both high and low superheat.
5. Write seminar for presentation on 13th June 2001.

If anyone has any suggestions or comments, please do not hesitate to get in contact: j.a.lawrence@gre.ac.uk



3D MESH 45deg


FEMGV 6.1-02 : University of Greenwich
29-MAY-2001 13:39 report1
Model: CASEFW
Analysis: PHYSICA
1
2
3

3D geometry

INFORM FILE

```
# Free surface mold filling
# James Lawrence
# University of Greenwich
#
GEOMETRY_MODULE
  FILENAME casefw
  GRAVITY_Y -10.0
END

GENERIC_MODULE
  TRANSIENT_RUN
    DELTA_T
      USER_DELTA_T
      FOR_ALL_TIME_STEPS 0.0005
    END
    END_TIME 2.00
    SAVE_AT_EVERY_TIME_STEP -1
  END
  MAX_SWEEPS 30
END

MONITOR_MODULE
  OUTPUT_INTERVAL 10
  FRACTION_DIGITS 5
  BLOCK_FORMAT ON
END

POST-PROCESSING_FORMAT
  FEMGV_FORMAT
    SET_FEMVIEW_WRITE 10
  END
END

FREE_SURFACE_MODULE
  EXPLICIT_FACTOR 1.0
# CONVECTION_METHOD DONOR_ACCEPTOR
  CONVECTION_METHOD VAN_LEER
  EXPLICIT_SOLUTION_STAGE START_OF_TIME_STEP
  GALA ON
  SOLVE_FREESURF
    INITIAL_VALUES USER_ROUTINE perpatch 2 0.0 1.0
  END
# BOUNDARY_CONDITIONS
#    PATCH 1 FIXED_VALUE VALUE 1.0
```

```
# END
END

MATERIAL_PROPERTY_MODULE
  DENSITY
    MATERIAL 1 USER_ROUTINE FS_PROP 2 1000.0 1.0
    SAVE_PROPERTY END_OF_RUN
  END
  VISCOSITY
    MATERIAL 1 CONSTANT 0.0 1.0E-08
  END
END

FLUID_FLOW_MODULE
  BUOYANCY
    REFERENCE_DENSITY 1.00
  END
  SOLVE_U-MOMENTUM
    INITIAL_VALUES ALL 0.0
#     BOUNDARY_CONDITIONS
#     PATCH 3 WALL COEFF 1.0 VALUE 0.0
  END
  SOLVE_V-MOMENTUM
    INITIAL_VALUES ALL 0.0
#     BOUNDARY_CONDITIONS
#     PATCH 3 WALL COEFF 1.0 VALUE 0.0
  END
  SOLVE_W-MOMENTUM
    INITIAL_VALUES ALL 0.0
  END
  SOLVE_PRESSURE
    INITIAL_VALUES ALL 0.0
    BOUNDARY_CONDITIONS
      PATCH 5 FIXED_VALUE VALUE 0.0
      PATCH 2 FIXED_VALUE VALUE 0.0
    END
  END
END

STOP
```

Document # 6
Name: James Lawrence
Title: Steady 1D Convection diffusion (Upwind)
Date: 03.12.01

Introduction

This problem is outlined on page 116 of An Introduction to Computational Fluid Dynamics The Finite Volume Method By HK Versteeg and W Malalasekera. A steady state convection - diffusion problem is solved using the upwind differencing scheme in one dimension. The grid used is a coarse 5 point grid(1) and compared to the analytical solution. The purpose of this is to build up a framework that can be used for different problems using different differencing schemes. The framework can then be modified to be used in more than one dimension.

Case 1 One dimensional convection steady convection diffusion

This problem is solved using the upwind differencing scheme and is a test problem from page 116 of An Introduction to Computational Fluid Dynamics The Finite Volume Method By HK Versteeg and W Malalasekera. The grid used is shown below in fig.1.

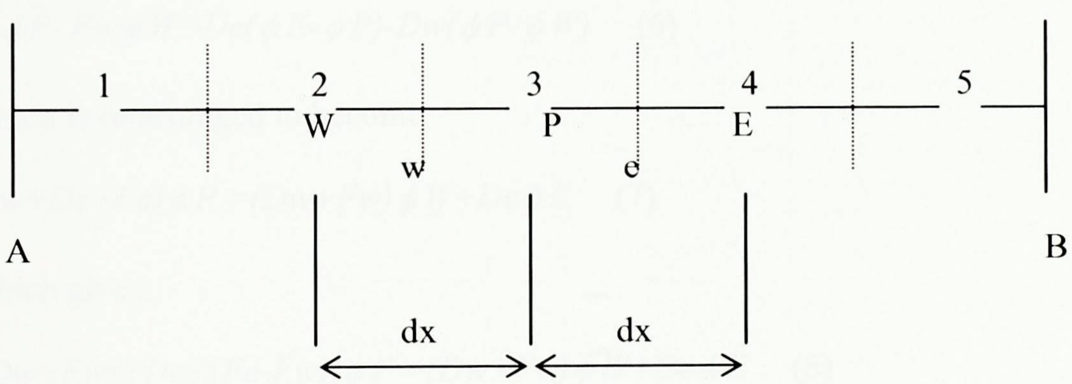


fig. 1 Case 1 Computational grid

For this example the governing equation is as follows:

$$\frac{\partial(\rho u\phi)}{\partial x}=\frac{\partial}{\partial x}\left(K\frac{\partial\phi}{\partial x}\right) \quad (1)$$

Where, ρ=1, u=0.1, ∂x=0.2 and K=0.1. The boundary values of ϕ at A and B are 1 and 0 respectively.

Following the usual practice for the integration of the governing equation the discretised equations become the following:

$ap\phi p = aW\phi W + aE\phi E + Su$ (2)

Where,

$ap = aW + aE + (Fe - Fw) - Sp$ (3)

If we back track for a moment we can see how the discretised equations were formed by use of the upwind differencing scheme. It is especially useful to look at how the equations were formed at the boundary nodes 1 and 5.

By use of upwind differencing for the convective terms we obtain:

Boundary 1:

$Fe\phi P - FA\phi A = De(\phi E - \phi P) - Dw(\phi P - \phi A)$ (4)

Boundary 5:

$FB\phi P - Fw\phi W = DB(\phi B - \phi P) - Dw(\phi P - \phi W)$ (5)

For generic internal nodes (2,3and 4) the equation is:

$Fe\phi P - Fw\phi W = De(\phi E - \phi P) - Dw(\phi P - \phi W)$ (6)

Which is re-arranged to become,

$(Dw + De + Fe)\phi P = (Dw + Fw)\phi W + De\phi E$ (7)

Which gives,

$((Dw + Fw) + De + (Fe - Fw))\phi P = (Dw + Fw)\phi W + De\phi E$ (8)

$D = De = Dw = K/\partial x$ and $F = Fe = Fw$ everywhere, except at the boundaries $Da = Db = 2K/\partial x = 2D$

We are now in a position to collect terms for each node involved on the grid. This is best done in the form of a table for nodes 1 to 5.

Node	aW	aE	Sp	Su
1	0	D	-(2D+F)	(2D+F)ϕ
2,3,4	D+F	D	0	0
5	D+F	0	-2D	2DϕB

Once the coefficients have been calculated a matrix can be constructed and solved. The matrix for this problem is shown below.

AW	aP	aE	Su
0	0	0	0
0	1.6	-0.5	1.1
-0.6	1.1	-0.5	0
-0.6	1.1	-0.5	0
-0.6	1.1	-0.5	0
-0.6	1.6	0	0
0	0	0	0

This matrix is then solved by using the tri-diagonal matrix algorithm or TDMA by way of a computer program.

Results

Node	DX	FV	ANL sol	% error
1	0.1	0.933	0.9387	0.53
2	0.3	0.787	0.7963	1.05
3	0.5	0.613	0.6224	1.51
4	0.7	0.403	0.4100	1.68
5	0.9	0.151	0.1505	-0.02

The results for thi analytical solution which is given by:

$$\frac{\phi-\phi_0}{\phi_L-\phi_0} = \frac{\exp(\rho u}{\exp(\rho u}$$

Discussion

The upwind scheme is used as it identifies the flow direction. This is obviously useful in a highly convective flow. This scheme uses consistent expressions to calculate fluxes through cell faces which means the formulation is conservative. The scheme also accounts for flow direction, therefore the formulation has transportiveness built into it. In the one dimensional case the upwind scheme works well, but when the scheme is extended to two dimensional problems errors can occur when the flow is not aligned with grid lines. This produces smearing or false diffusion.

Conclusion

Scheme successfully constructed and tested.

Program

```
C
C**********************************************************
C  1D Convection (Steady Upwind)
C  James Lawrence
C  University of Greenwich
C  23/02/01
**********************************************************
**********************************************************
C  Title


C  Declaration of variables
      INTEGER I, J, Ncells, M
          REAL SP(7), AE(7), AP(7), AW(7), K, DX, RC, XSEC, A(7)
          REAL SU(7), Phi(7), C(7), Cdash(7), U, Rho, D, F
C  Input variables to ask for
      Ncells=7
      PRINT *, 'What is Delta T?'
C         READ *, DT
          PRINT *, 'What is u?'
          READ *, U
          PRINT *, 'What is the value of Rho?'
      READ *, Rho
          PRINT *, 'K value?'
          READ *, K
          PRINT *, 'DX value?'
          READ *, DX
      PRINT *, 'What is boundary phi 1?'
          READ *, Phi(1)
          PRINT *, 'What is boundary phi 2?'
          READ *, Phi(Ncells)
```

```
    D=(K)/(DX)
        F=Rho*U

        PRINT *, F
        PRINT *, DA
C  Initilialise A and Cdash to take account of boundary values
    A(1)=0.
        Cdash(1)=Phi(1)
        A(Ncells)=0.
        Cdash(Ncells)=Phi(Ncells)

        SP(2)=-((2*D)+F)
        SP(Ncells-1)=-2*D
C    PRINT*, SP(Ncells-1)

        AW(2)=0
C       PRINT*, AW(2)
        AW(Ncells-1)=(D+F)
C    PRINT*, AW(Ncells-1)

        AE(2)=D
C       PRINT*, AE(2)

        AE(Ncells-1)=0
C       PRINT*, AE(Ncells-1)

        AP(2)=AW(2)+AE(2)-SP(2)
C       PRINT*, AP(2)

        AP(Ncells-1)=AW(Ncells-1)+AE(Ncells-1)-SP(Ncells-1)
C       PRINT*, AP(Ncells-1)
C       PRINT*, '************************************************************'
        SU(2)=((2*D)+F)*Phi(1)
    SU(Ncells-1)=(2*D)*Phi(2)

C  This do loop is for the new source term 0 cos no source term
    DO I=3,5
```

```
          SU(I)=0
          END DO

      DO I=3,5
          SU(I)=0
          END DO

C  This do loop calculates AE, AP, and AW for each NODE
      DO I=3,5
          AE(I)=D
          AW(I)=(D+F)
          AP(I)=AW(I)+AE(I)-SP(I)
          END DO
C  This is necessary to fill up the matrix
      DO I=2,6
          AE(I)=-AE(I)
          AW(I)=-AW(I)
          END DO
C  This is filling up the matrix
          PRINT *, '    AW       AP       AE       SU'
          DO I=1,Ncells
          PRINT*,   AW(I), AP(I), AE(I), SU(I)
          END DO

C  This part chooses the solver
C     PRINT *, 'Choose solver: JACOBI(1) or TDMA(2)'
C
C         READ (*,*) IS
C         IF (IS.EQ.1) THEN
C           CALL JACOBI(Ncells,AE,AP,AW,SU,Phi,PhiNew)
C         ELSEIF (IS.EQ.2)
C           CALL TDMA(Ncells,AE,AP,AW,SU,Phi,A,Cdash)
C     END IF
C     END
C  This do loop now calculates all the A and Cdash values
C     SUBROUTINE TDMA(Ncells,AE,AP,AW,SU,Phi)
C         INTEGER Ncells,I
C         REAL AE(7),AP(7),AW(7),SU(7),Phi(7)

C     DO
          C(2)= 1.1
          DO I=3,6
          C=0
          END DO
```

```
      DO I=2,Ncells-1
      A(I)=(-AE(I))/(AP(I)+(AW(I)*A(I-1)))
      Cdash(I)=((-AW(I)*Cdash(I-1))+SU(I))/(AP(I)+(AW(I)*A(I-1)))
      PRINT*, A(I)

      PRINT*, Cdash(I)
C     PRINT*, '****************'
      END DO

C This loop does the backwards substitution

      DO J=6,2,-1
      Phi(J)=A(J)*Phi(J+1)+Cdash(J)

   PRINT*, '****************'
      PRINT*, Phi(J)
      PRINT*, '****************'
      END DO


      END


C This is the Jacobi Subroutine
C     SUBROUTINE JACOBI(Ncells,AE,AP,AW,SU,Phi,PhiNew)
C       INTEGER Ncells,J,I
C       REAL AE(7), AP(7), AW(7), SU(7), Phi(7), PhiNew(7)


C       DO J=1,100
C         DO I=2,Ncells-1
C         PhiNew(I)=((SU(I)-(AW(I)*Phi(I-1))+(AE(I)*Phi(I+1)))/AP(I)
C         END DO

C         DO I=1,Ncells
C         Phi(I)=PhiNew(I)
C         END DO
C     END DO
C       PRINT *, Phi(I)

C       RETURN
```

Document # 7
Date: 29/11/01
Name: James Lawrence
Title: Thesis Plan / Work Plan of action

Aim

The aim of this document is to produce a plan of action as far as possible for work to be carried out and how this is to be presented in the future. Ultimately this should be a list of reachable goals and achievements together with an idea of how to present these goals and achievements. In order to do this it is useful to start with an ultimate goal. This being the main reason behind the project.

Overall Objective

The rough overall aim of this project as now stands is to produce a fully working transient 3D model of the pouring and solidification of the pouring of a Ti-Al alloy casting. This model will be used to predict bubble entrapment and porosity. In order to do this a free surface model is to be produced that does not suffer from numerical diffusion and accurately captures the liquid - air interface during pouring. His free surface model is to be produced using the CIP method as produced by Yabe et al. This accurate free surface can then be used to model bubble formation due to surface turbulence.

Plan of Action

- Produce 1D models of steady convection diffusion equations from Versteeg examples (whatever differencing technique).
- Produce 1D transient models using different differencing techniques, such as upwind, central difference, QUICK etc of the advection equation. This is to be done explicitly and implicitlty.
- Produce multidimensional models of stage 2.
- Produce 1D transient CIP model.
- Produce CIP model in multidimensional form.

This plan only outlines the necessary test work to be carried out before the model can be implemented into PHYSICA. A separate document will be produced for this stage of work.

Writing Thesis

An hour is to be spent each day on writing up the test cases. These are then to be kept in a file and used as a reference when writing up the final version.

Each test case will be written up in the following lose form.

- Aim
- Purpose
- Method
- Results
- Discussion
- Conclusion

These test cases will be filed in order and will serve as a useful reminder along with a lab book and other literature and reports that are to be read or produced.

Document # 8
Implementation of Various Differencing Schemes into PHYSICA
James Lawrence
07/01/02

SUMMARY

This document outlines the method for the implementation of various differencing schemes into the PHYSICA multi-physics software package. The method is drawn from a variety of sources including existing literature and programming documentation. This report is to serve as a guide that can be used as a reference in the future as no satisfactory documentation exists at this time. It will also be used as an historical record of how the technique is developed over a period of time. Two major strategies are used to achieve the discretization of the governing equations. These techniques are known as Flux Limiters (FL) and Normalized-Variables (NV). As far as this study goes at this moment in time the Flux Limiter technique is focused on

INTRODUCTION

Although methods of calculating free-surfaces exist within PHYSICA at this time, these methods tend to suffer from numerical diffusion (non-physical diffusion) to varying degrees which renders problems inaccurate and sometimes completely useless. A constant battle is being fought to find a method that provides a sharp resolution of the free-surface as well as accuracy and good solution behaviour. The main aim of this is to provide an accurate model of the free-surface when considering the pouring of a metal casting where the turbulent free-surface is directly related to bubble entrapment which in turn leads to poor quality castings. This is especially important when considering high integrity components such as turbine blades and turbocharger rotors.

Only the convection conservation equation is considered here, which is governed by the following equation,

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}=0 \qquad (1)$$

In one-dimension this can be shown to be the simple translational motion of a wave when u is constant. The value and position of certain points in the wave relates in some respects to a free surface, but the hope is to convert the model to three dimensions.

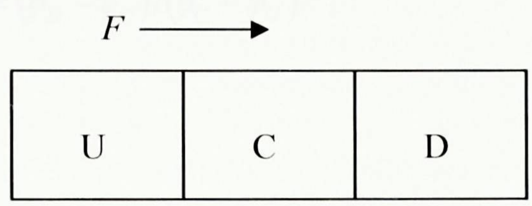
The main reference used in this implementation is the paper by Waterson and Deconink (1), which outlines a unified approach to the design and application of bounded higher-order convection schemes. Before transient problems such as that shown in equation (1) are considered, the same problem in the steady state is considered.

$$u\frac{\partial f}{dx} = 0 \qquad (2)$$

The finite volume discretization can be for a cell may be generalised as:

$$a_p\phi_p = \sum {}_{nb} a_{nb}\phi_{nb} \qquad (3)$$

Cell face values are calculated using the upwind-biased framework shown below.



Linear schemes are expressed as members of the convenient calss of Kappa schemes. The cell-face valueof the convected variable may be written as the first order upwind scheme with an additional *"anti-diffusive"* term.

$$\phi_f = \phi_C + \{ \tfrac{1}{4}(1-k)(\phi_D - \phi_C) + \tfrac{1}{4}(1-k)(\phi_C - \phi_U) \qquad (4)$$

The value of Kappa is dependent on the particular upwind scheme being used some typical values are

K=1 Central Difference
K=1/2 QUICK
K=1/3 Cubic upwind
K=0 Fromms Scheme
K=-1 Linear upwind

NON-LINEARSCHEMES: FLUX LIMITER APPROACH

The way in which this scheme is developed is to generalise the Kappa scheme shown in equation (4).

$$\phi_f = \phi_C + \tfrac{1}{2}B[(\phi_D - \phi_C),(\phi_C - \phi_U)] \qquad (5)$$

The function B(p,q) is designed to give higher order accuracy where possible ensuring boundedness conditions are satisfied. It is more convenient to write (5) as,

$$\phi_f = \phi_C + \tfrac{1}{2}\psi(r)(\phi_C - \phi_U) \tag{6}$$

where $\psi(r) = B(r,1)$. This is termed the limiter function, where the gradient ration r is defined as:

$$r = (\phi_D - \phi_C)/(\phi_C - \phi_U) \tag{7}$$

Document # 9

BUBBLE DEFECT DEVELOPMENT AND DISRIBUTION IN THE CASTING OF PURE ALUMINIUM AND AN ALUMINIUM BASED ALLOY

James Lawrence

05.02.02

INTRODUCTION

At certain critical velocity values the turbulent surface of a liquid metal being cast becomes extremely unstable. The result of this is dross inclusion and bubble formation from entrained oxide films and air within the mould. This leads to subsequent damage to the integrity of the casting. This severely impairs component performance and therefore it is essential that such defects are minimised or preferably eliminated improving the mould filling and thus the quality of the castings. In order to achieve this care needs to be taken over the design of the running system and the method chosen to pour the metal. Traditionally this has been done in a trial and error fashion. However, Casting trials can prove expensive, non repeatable and time consuming, therefore a tool is being developed at the University of Greenwich that will enable the prediction bubble defects within castings using a numerical approach. This will enable running systems and pouring techniques to be designed and assessed without the construction of the full casting system.

This report describes some of the initial experimental work carried out at the University of Birmingham to investigate the development and propagation of bubble defects in sand castings of pure Aluminium and 2L99 at varying superheats. The purpose of this work was to point modelling in the right direction so far as the distribution of bubble defects is concerned. The sand moulds were built on site at the University of Birmingham where they were subsequently poured. The distribution and development of the bubble defects was monitored using real time X-ray radiography (fig.1). A number of the casting conditions were repeated and tested for reproducibility, which is useful from the point of view of model validation.

The casts were successful and some degree of repeatability was achieved. However, taking into account the random nature of the flow and slight variations in the mould geometry, sprue geometry, running systems and pouring conditions it will not be possible to use the repeated tests as definitive validation experiments. It is therefore recommended that further work be carried out when in a position to validate the model. However, the results from the experiments will be useful as a guide in the model development.

There is a limited amount of literature that includes detailed analysis of bubble formation in castings. It is generally agreed that the formation of bubbles and the inclusion of dross is closely related to the condition of the free-surface of the liquid metal being poured. The main aim of running systems with regard to this is to induce a laminar flow of the liquid metal upon entry to the ingate of the mould. However when considering bubble mechanisms life is not quite this black and white. It was suggested by Eastwood in the 1940's that there are two types of turbulence present in filling situations.

1. **Surface Turbulence:** This is the situation where the turbulence is so severe that the oxide skin around the periphery of the flowing metal is broken and the surface skin is distorted or ruptured, which leads to bubble formation or dross inclusion
2. **Bulk Turbulence:** This is a less severe form of turbulence which does not break or dangerously distort the oxide film.

When considering bubble formation surface turbulence is the main cause and is influenced by a critical value of velocity. This is demonstrated by way of a simple model (fig.1).

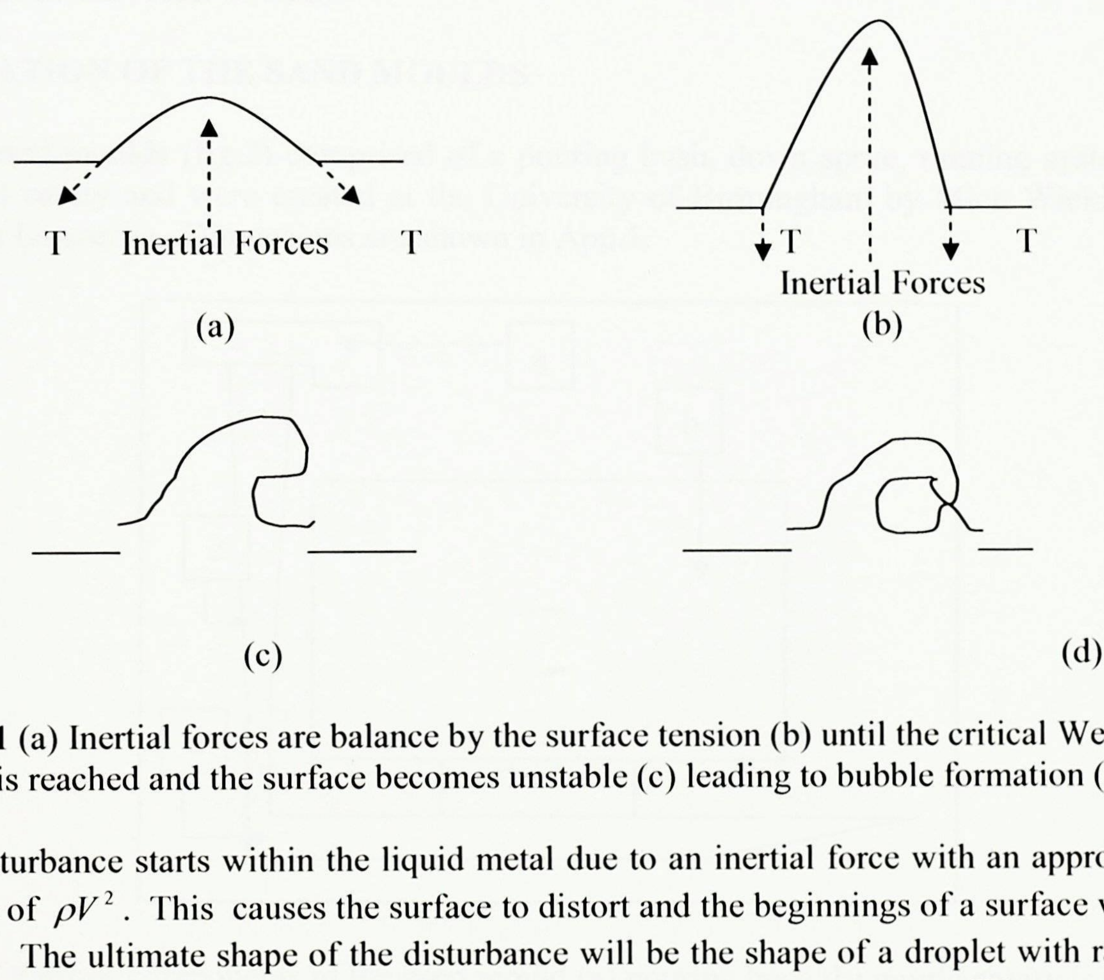


Fig.1 (a) Inertial forces are balance by the surface tension (b) until the critical Weber no is reached and the surface becomes unstable (c) leading to bubble formation (d)

A disturbance starts within the liquid metal due to an inertial force with an approximate value of ρV^2. This causes the surface to distort and the beginnings of a surface wave to form. The ultimate shape of the disturbance will be the shape of a droplet with radius r. A limiting condition can be seen to be when the surface tension force $\frac{2T}{r}$ is in balance with the inertial forces. At this point the surface can either break and dross inclusions can be created or the surface folds over on itself to create a bubble or crack. In the case of molten aluminium this phenomena can be severe as a dry oxide skin is without fail always present.

The balance of the two forces is shown as

$$\rho \times V^2 = \frac{2T}{r}$$

Therefore,

$$V_{crit} = \sqrt{\frac{2T}{r\rho}}$$

This shows a critical velocity at which there is a severe and very likely risk of some kind of bubble inclusion. The ratio of the internal forces to the surface tension force is known as the Weber number and is therefore a critical property that needs to be tracked for any kind of model that is to predict bubble defects.

EXPERIMENTAL WORK

CREATION OF THE SAND MOULDS

The sand moulds (fig.2) comprised of a pouring bush, down sprue, running system and mould cavity and were created at the University of Birmingham by Mick Wickins and James Lawrence. Dimensions are shown in App.1.

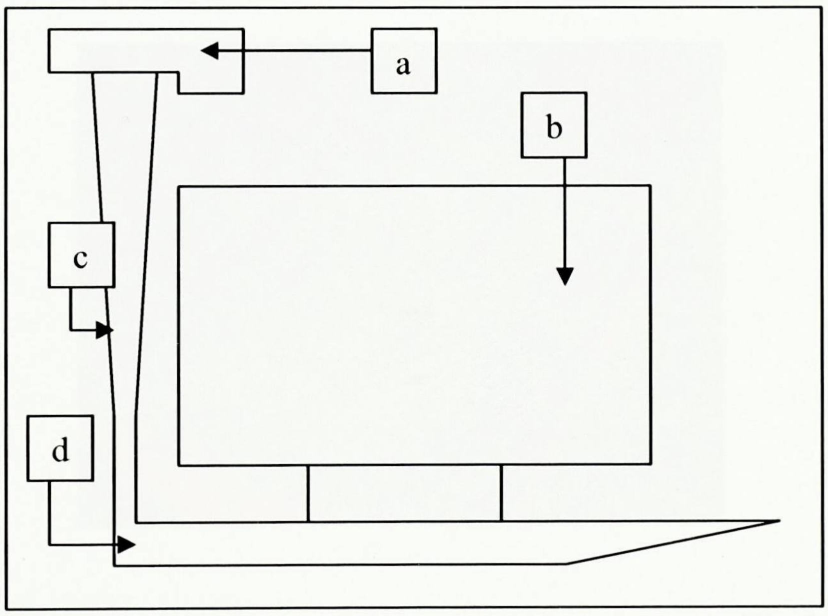


Fig.2 Various components of the sand mould (a) pouring bush (b) mould cavity (c) down sprue (d) running system.

250kg of grade 60 Silica sand was poured in to a mixing vessel and was mixed with PEPSET 5112 (an organic polyol dissolved in a solvent) and PEPSET 5230 (an isocyanate dissolved in a solvent) for around 2 minutes. The PEPSET 5000 series is a 2 part pre-catalysed binder and was used in the proportion of 1.2% by weight (0.6% of each part) of binder to sand.

The sand / binder mixture was then used to fill the wooden pattern (fig.3) and left to harden in the for around 15 minutes.

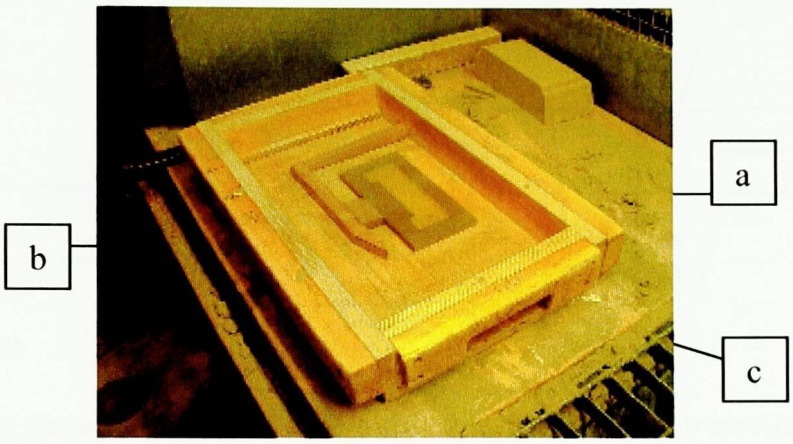
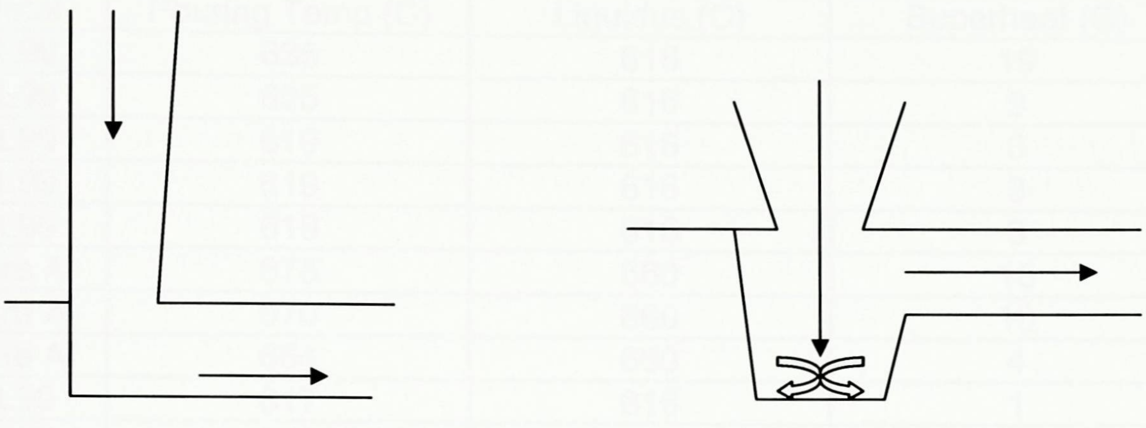


Fig.2 Wooden mould pattern which comprises of the downsprue (a) the running system (b) and the mould cavity (c). A pattern was also available for the pouring bush and the back of the mould

Once sufficiently hard the various parts sand moulds were beaten out of the pattern and stored (fig.3). 11 moulds were created altogether allowing for pouring at varying superheats and repeatability tests.

Fig.3 Mould produced from the pattern shown in **Fig.2**.

The moulds were created with a thick section runner (fig.4) encouraging the development of bubbles within the system, which provided sufficient data to be studied.



(a) (b)

Fig.4 Bad running system design (a) where splashes occur in the transition from the sprue to the runner. A better design of running system (b) avoiding splash effects in the transition from sprue to runner.

POURING AND REAL TIME X-RAY VIDEO

In order to gain some useful results real time x-ray video footage was collected as the molten aluminium and alloy were poured. This enabled the development and propagation of the bubble defects to be monitored and output to VHS tape. Subsequent playback enables modelling work to be directed by the practical results which act as a benchmark. This is available from James Lawrence or Mick Wickins.

EXPERIMENTAL PROCEDURE

The mould was assembled (comprising of the pouring bush, down sprue, runner and mould cavity) and a charge of metal (pure Al or 2L99) was melted in a crucible. The liquidus of each metal is well exceeded in the crucible to give adequate time before the appropriate superheat is reached. The temperature was measured by a calibrated thermocouple. The cooling curves are available for this (App.2). The hot crucible is loaded into a remotely operated pouring mechanism, which is monitored from the control room.

RESULTS AND COMMENTS

Varying superheats were used with two different metals and the effect this had on the production and propagation of bubbles was recorded (fig.5).

Metal	Pouring Temp (C)	Liquidus (C)	Superheat (C)
2L99	635	616	19
2L99	625	616	9
2L99	619	616	3
2L99	619	616	3
2L99	619	616	3
Pure Al	678	660	18
Pure Al	670	660	10
Pure Al	664	660	4
2L99	617	616	1
2L99	619	616	3
2L99	625	616	9

Fig.5 Various superheats with the alloy 2L99 and commercially pure Aluminium

The different conditions used provided a good range of superheat, which means the effect of varying superheat on bubble activity in the different alloys can be assessed. This is best done by looking at the real time x-ray video footage as this shows the both the turbulent filling and subsequent bubble formation.

CONCLUDING REMARKS AND DISCUSSION / MODELLING METHODS

At this stage it is necessary to look at a possible technique to model the movement of bubbles within the molten metal. Work has been done in the past to model bubble formation in the continuous casting process of some **kinda metal**. The dimensions of these bubbles are insignificant compared to the size of the bubbles created in the Aluminium castings, the former being an extreme sub-cell size. The usual method is to model the bubble movement using particle tracking techniques. The particle centre is usually tracked over time and this has been done with a good degree of success (say who's dunnit). But when the particle spans more than one cell (as in Aluminium) they are all affected. There is then the question of how much of the bubble is in each cell. This is needed to firstly get a representative value of the continuum quantities, and than decide how much of the source is to be added.

(a) (b)

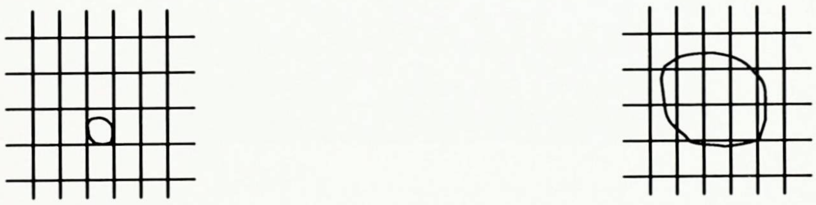


Fig.6 (a) sub-cell particle dimensions and (b) particle covering multiple cells

There are also problems as particle tracking is computationally expensive in terms of both CPU time and storage requirements.

Free-surface techniques have an advantage over the tracking techniques where bigger bubbles are concerned. They are efficient and computationally inexpensive. The algorithms and tools already exist in PHYSICA also which allow voids to be modelled in two phase free surface problems where the surface wraps over itself. However, the problem remains of how to predict whether the bubble will escape from the geometry or whether the will end up as an inclusion of the final component. The way in which this will be done is to find a sink term which can be added to the momentum equations which restricts the motion of the bubbles within the molten metal.

Document # 10

Name:	James Lawrence
Date:	20/02/02
Title:	LSM based surface tension modelling using PHYSICA

The following document is a list of validation tests that are to be carried out to assess the ability of PHYSICA to model surface tension using the Level Set Method (LSM). There are certain benchmark tests carried out and some special cases that are related to bubbles and droplets, which are a result of surface tension phenomena.

Test 1

1. Introduction

Surface tension plays an important role in many fluids problems and industrial processes, such as welding, casting and solder join formation. Of particular interest is the formation and distribution of bubbles in metal casting causing the integrity of finished components to be compromised. This is directly related to surface tension.

The first test is the evolution of a 2D square into a circle due to the action of pure surface tension. Figure 1(a)shows the evolved circle. The structured grid contained 2500 elements and is shown in figure 1(b).

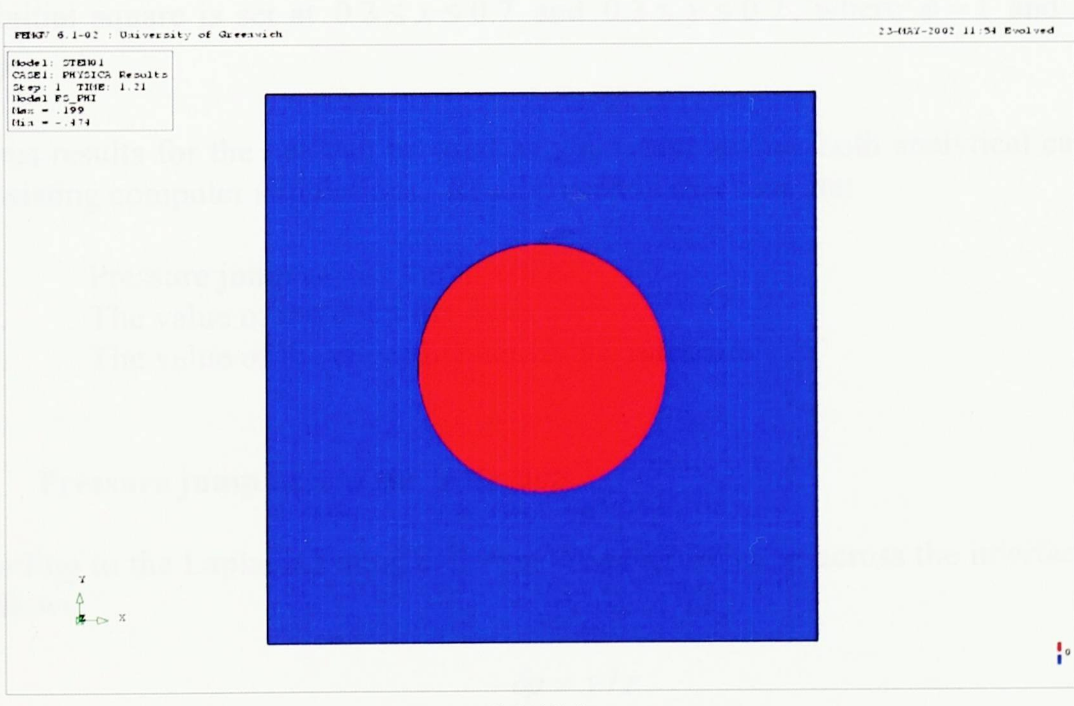


Figure 1(a): Original Square with

surface tension (0 level set).

Figure 1(b): Structured mesh containing 2500 elements.

The initial square is set at $0.3 \le x \le 0.7$ and $0.3 \le y \le 0.7$, where $\phi = 1$ and anywhere else $\phi = -1$.

Various results for the test can be used as validation against both analytical calculations and existing computer simulations. Results used in this case are:

1. Pressure jump across the interface.
2. The value of the delta function.
3. The value of the curvature across the interface.

2. Pressure jump across the interface

According to the Laplace-Young equation the pressure jump across the interface is given as follows:

$$\delta p = \gamma / r$$

Where γ is the value of constant surface tension unaffected by local temperatures and r is the radius of the evolved circle. In our test case the value of the constant γ is 10.0. The radius of the evolved circle is equal to 0.22. Therefore, the analytical pressure drop across the interface is equal to 45.45. The value obtained from the simulation is equal to 38.78.

The agreement between the pressure jumps for both the analytical result and the simulation is relatively good. The simulated values for the pressure field across the interface are shown in figure 2.

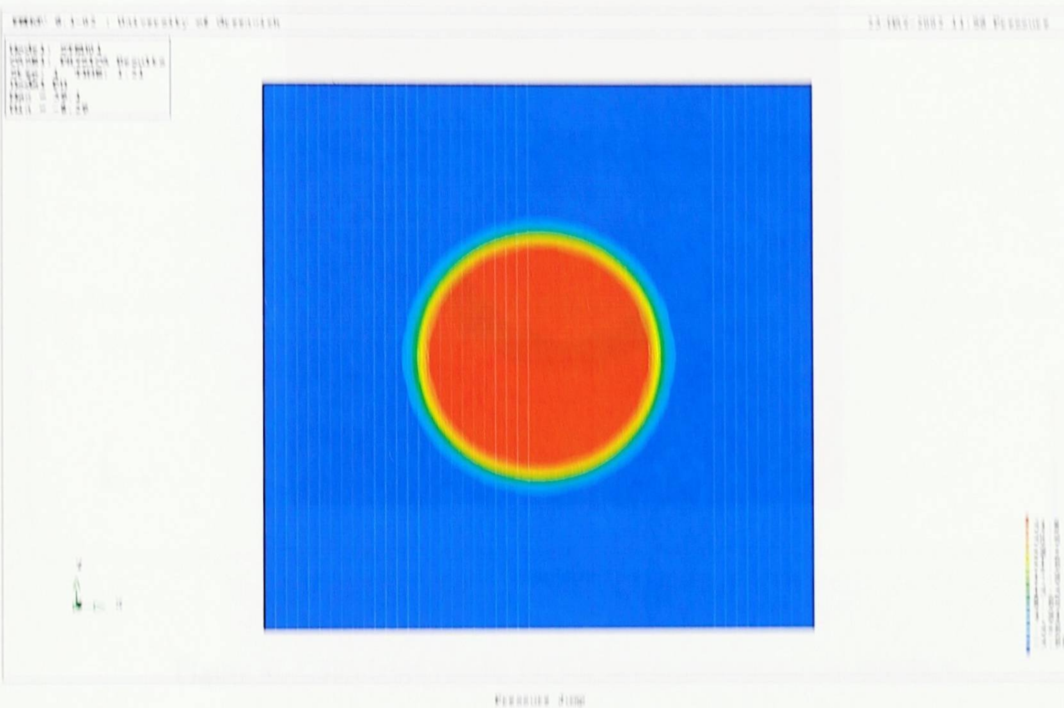


Figure 2: Pressure jump across Interface.

3. Value of the Delta Function

The delta function must be given such that $\int_{-\epsilon}^{\epsilon}\delta(\phi)d\phi = 1$ and confines sources to cells which lie near the interface. Values at the 4 points where the grid is at a tangent to the circle were obtained.????

4. Value of the Curvature across the interface

The value of the curvature was evaluated across the interface and approximate values between -2.78 and -5.11 were recorded. The required value is -4.43 (1). The calculated results for the curvature are shown in figure 4.

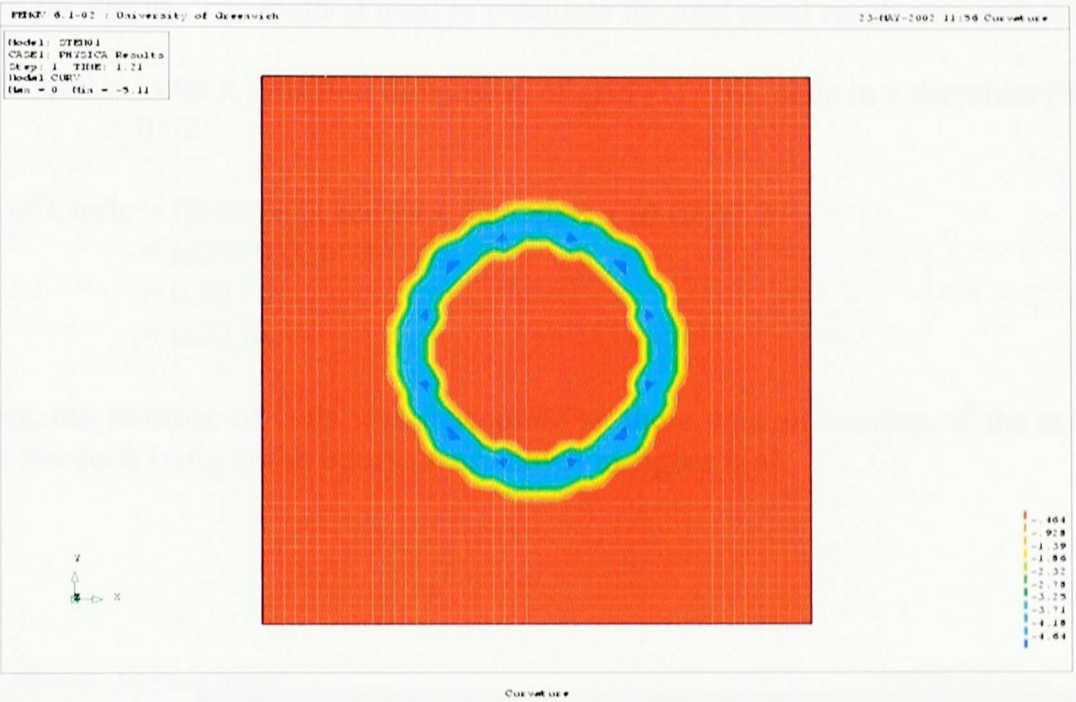


Figure 4: Calculated results for surface curvature across interface.

5. Comparison of Results

The results from the current study were compared with results obtained in a similar study (1). The purpose of this was to validate the new code against results that have already been validated

6. Conclusions

The comparison between the PHYSICA-2.12 and the previous version of PHYSICA (inc. surface tension) [1] showed the new code to be successful in predicting the evolution of a square into a circle purely by the act of surface tension. Comparisons of the results for interface pressure jump, delta function and curvature demonstrated this adequately. An extra comparison with analytical calculations also demonstrated the validity of the original results. Some error is present between the three sets of results. This error is due to a number of factors. Firstly, the difference in curvature values can be attributed to the curvature only being an estimate local to each cell neighbourhood, which is essentially an approximate sum over the faces of each cell given by:

$$J(\phi) = \left(\delta_{ij} - \frac{\phi_{xi}\phi_{xj}}{|\nabla \phi|^2} \right) \sum \frac{A_f (n_j)_f \left(\alpha_f (\phi_{xi})_A + (1-\alpha_f)(\phi_{xi})_P\right)}{V_P \left(\alpha_f |\nabla \phi|_A + (1-\alpha_f)|\nabla \phi_P|\right)}$$

The difference in pressure can be explained by inaccuracies in the measurement of the radius of the circle. The method used to calculate the analytical result was as follows:

Distance/cell = Total x direction dimension of grid (1) / No. cells in x direction (50)
= 0.02

Radius of Circle = ((No. cells across x diameter) x (0.02)) / 2
= (22 x 0.02) / 2
= 0.44 / 2
= 0.22 m

However, the number of cells was inaccurate as there was an overlap of the surface in some of the cells lying at the interface as shown in figure 6(a).

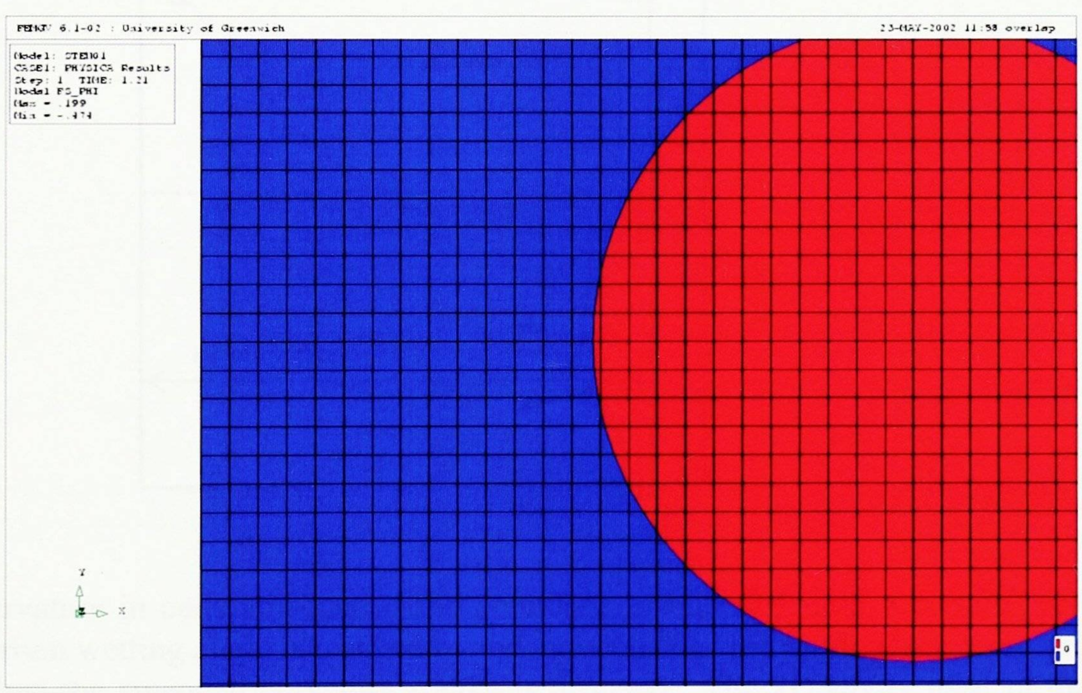


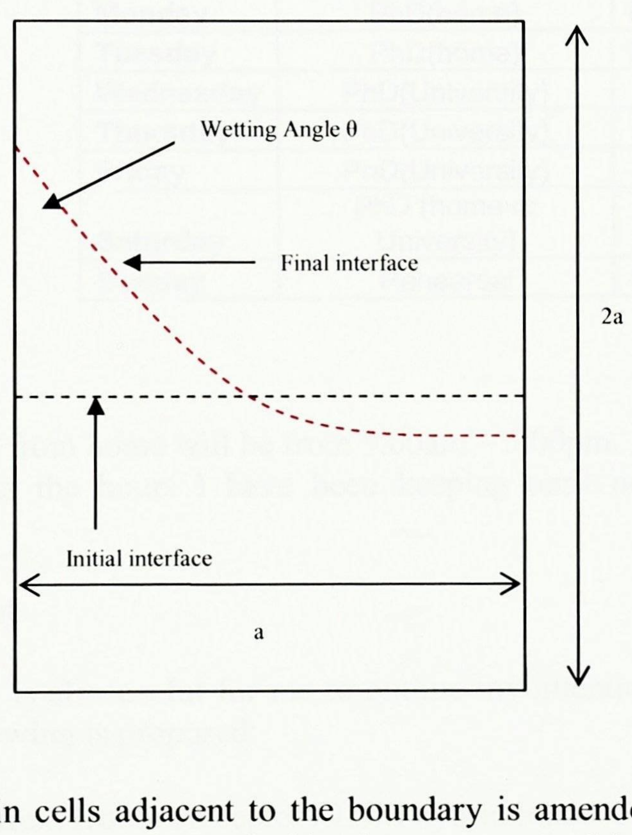
Figure 6(a): Showing overlap at interface leading to inaccurate dimension calculations.

However, as mentioned earlier the difference does not cause too much concern. The main aim here was to show that the code works for a specific validation case. The test demonstrates that the code is able to model the effect of pure surface tension ignoring any local temperature effects normally associated with surface tension phenomena.

Test 2

1. Introduction

When the interface between two fluids comes into contact with another external surface a force is exerted on the fluid. Due to the action of this force there is a subtle movement of the fluid. This is demonstrated below in figure 1(a).



The curvature in cells adjacent to the boundary is amended until a certain pre-defined equilibrium wetting angle is reached by the movement of the fluid. Once this equilibrium is reached the amended curvature source is dropped. The 2D cavity used in the test is shown in figure 1(a). The initial position of the interface is 90° to the boundary and the horizontal and vertical dimensions of the cavity are a and 2a respectively. The dashed red line in figure 1(a) shows how the shape of the interface is changed due to the addition of the extra surface.

Again the simulated results used to validate this test are the zero level set of ϕ, the delta function and the curvature.

Document # 12
Name: James Lawrence
Date: 02/09/02
Title: Proposed working schedule for 2002 / 2003

Timetable

The purpose of this document is to outline a work plan for 2002 / 2003 in order to continue with my PhD as well as continue with my musical activities.

I am proposing at this stage an arrangement that will involve me sharing my work between home and University enabling me to both study and rehearse. With this in mind I have created a timetable outlining my intentions. A typical week will consist of the following:

	Daytime	Evening
Monday	PhD(home)	Rehearsal
Tuesday	PhD(home)	Rehearsal
Wednesday	PhD(University)	
Thursday	PhD(University)	
Friday	PhD(University)	
Saturday	PhD (home or University)	
Sunday	Rehearsal	Rehearsal

Working hours from home will be from 9.00am – 5.00pm. Work hours at University will be the same as the hours I have been keeping until now (approximately 9.00am – 6.00pm).

Work Proposal

At this point it is also useful for me to outline my intentions for the next 6 months to a year. The following is proposed:

- Test current Donor Acceptor / LSM hybrid model for actual physical resemblance. This will involve testing at different Weber numbers and observing the response of the model.
- Create three dimensional model of the cast plate from Birmingham and test against lab results.
- Write up results and findings.
- Test model on more complex geometries / components.

CFD Modelling of Bubble Entrainment in TiAl Castings

By James Lawrence

Supervisors: K.A. Pericleous
R.A. Harding
V. Bojarevics

Interdisciplinary Research Centre THE UNIVERSITY OF BIRMINGHAM

the UNIVERSITY of GREENWICH

EPSRC

Presentation Format

- Casting Fundamentals
- Bubble Defects
- Filling of Castings with PHYSICA
- Physics of Bubbles
- Level Set + Surface Tension
- The Hybrid LSM + Donor-Acceptor model
- Results and Validation
- Conclusions/Suggestions

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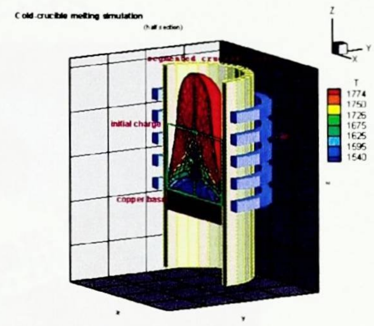
Casting Fundamentals

- Metal Charge is Heated and Melts
- Molten Metal is Poured into a mould
- Mould Fills
- Solidification takes Place
- Range of Engineering Components Produced
- Defect-free components needed for Aerospace components



ISM Melting Process

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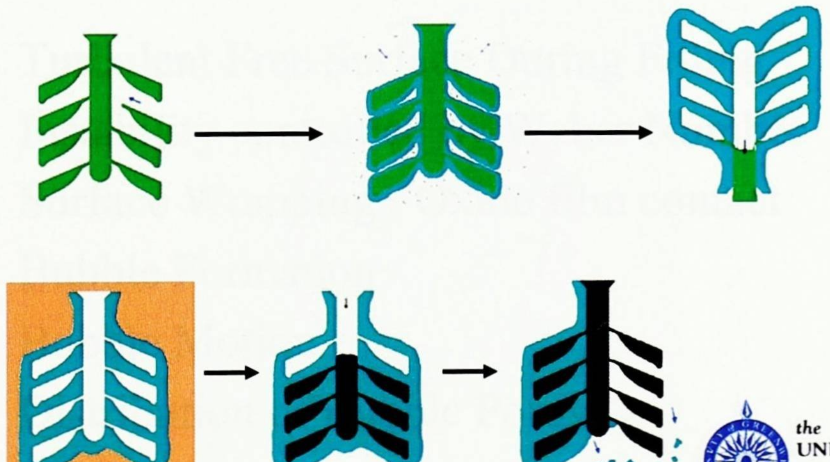
Investment Casting Schematic



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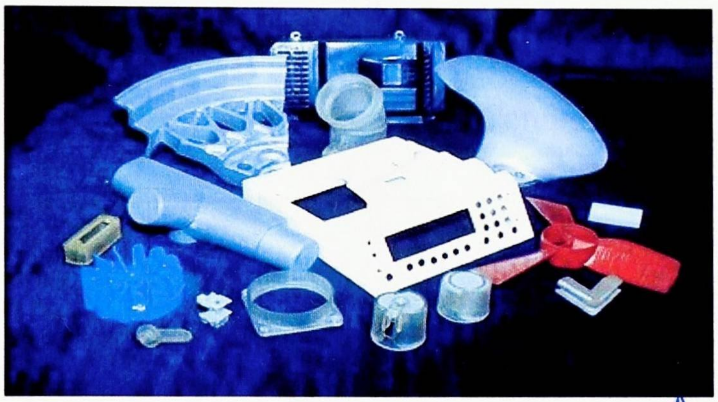
A Range of Engineering Components



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Bubble Defects

- Turbulent Free Surface During Filling
- Instability controlled by Weber Number
- Surface Wrapping / Oxide film contact
- Bubble Formation
- Bubble Motion
- Distribution of Bubble Porosity

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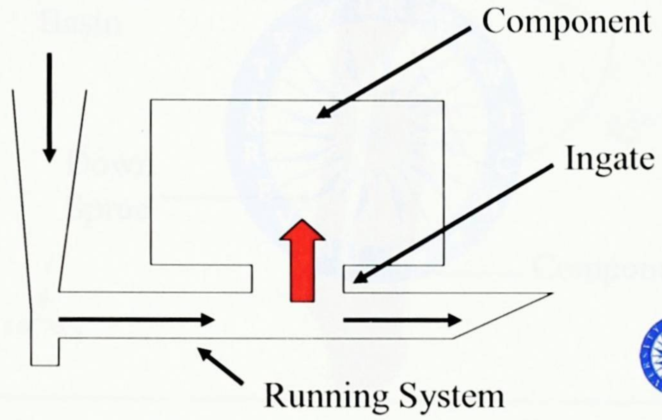
Running Systems

- Induce a Laminar Flow Before Ingate Entry



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Metal Pouring & Filling

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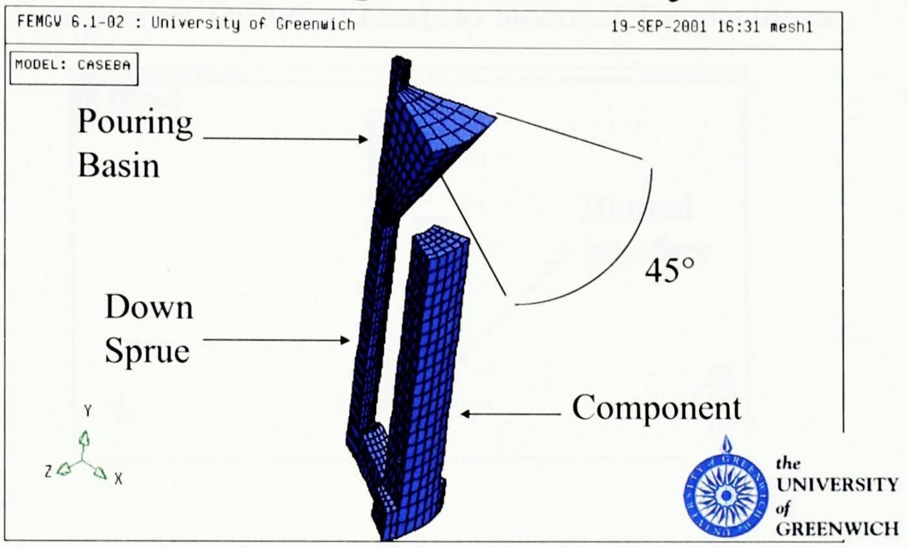
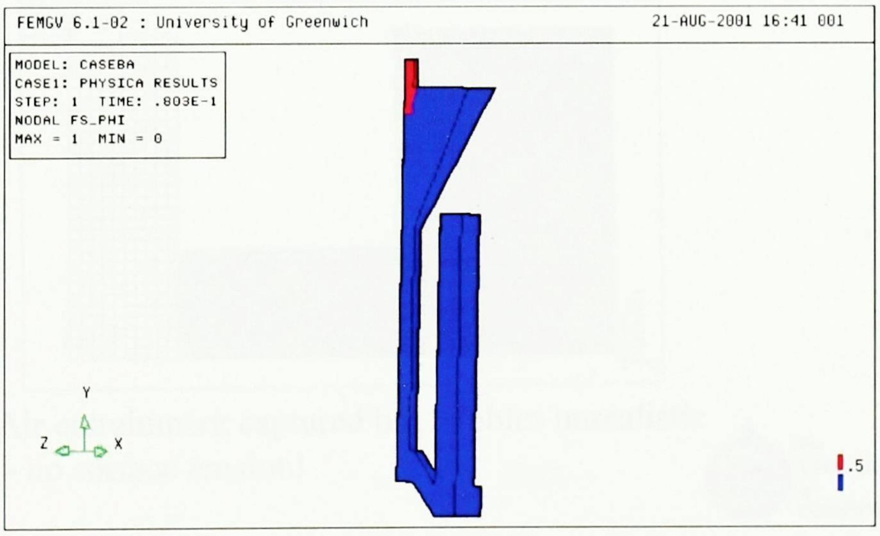
Meshing / Geometry

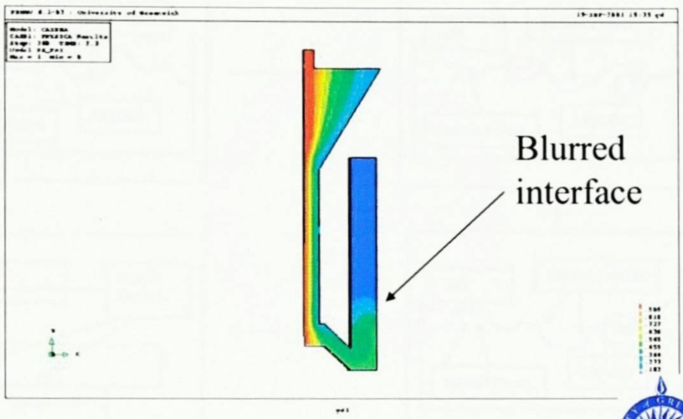


Results: 3D Mould Filling with Heat Transfer Animation



Physical / Numerical Problems

Free Surface Diffusion Leads to Incorrect Temperatures



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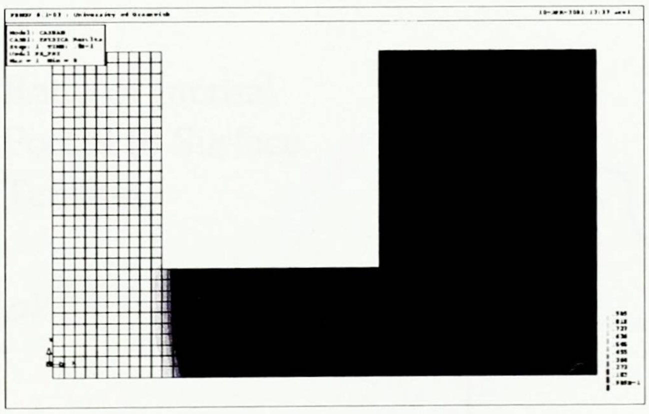
Results: 2D Filling Test Case animation



Air entrainment captured but bubbles unrealistic
- no surface tension!

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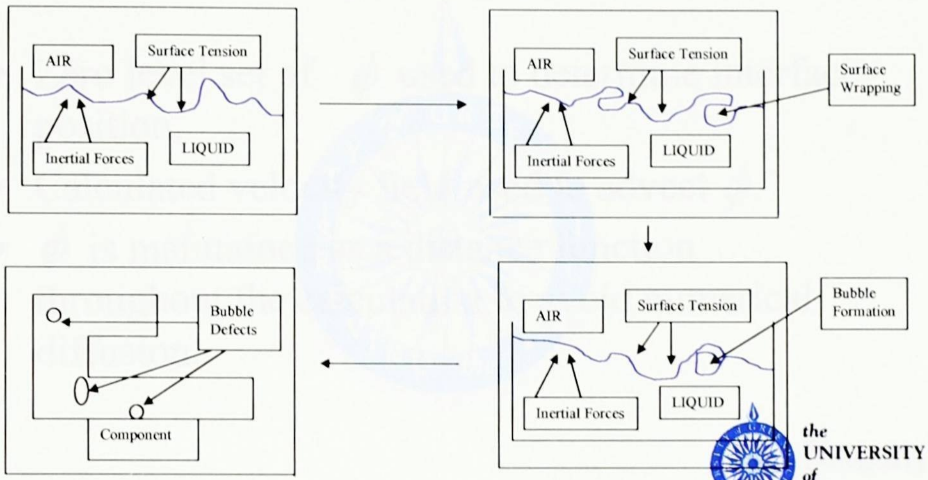
Examine Bubble Formation



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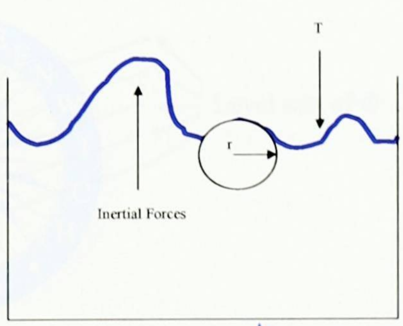
Weber Number

- Ratio of Inertial Forces to Surface Tension

$$\rho V^2 = \frac{2T}{r}$$



T = *Surface Tension* r = *Droplet Radius*
ρ = *Density* V = *Velocity*

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Surface Tension Modelling

(Level Set Method)

- Zero level set of ϕ used to determine interface position.
- Calculated velocity field used to advect ϕ.
- ϕ is maintained as a distance function throughout the calculation to avoid numerical diffusion.

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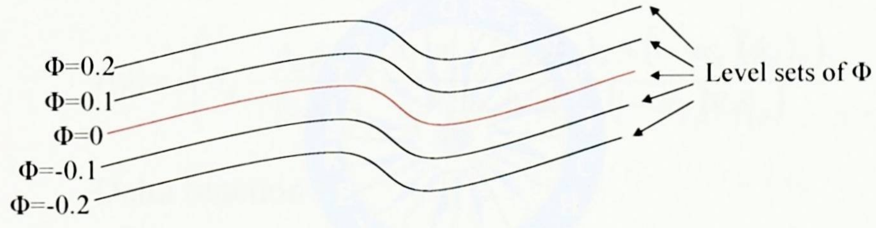
Level Set Method



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Surface Tension Modelling

(Level Set Method)

$$S_\gamma = \delta(\phi)|\nabla\phi|\nabla\gamma - \frac{\delta(\phi)}{|\nabla\phi|}(\nabla\phi.\nabla\gamma)\nabla\phi + \gamma\nabla\phi J(\phi)\delta(\phi)$$

$\delta(\phi)$ Delta function

$\nabla\phi$ Grad phi

$\nabla\gamma$ Surface tension grad

$J(\phi)$ curvature

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Surface Tension Modelling

(Level Set Method)

Curvature

$$J(\phi) = -\left(\delta_{ij} - \frac{\phi_{xi}\phi_{xj}}{|\nabla\phi|^2}\right)\Sigma\frac{A_f(n_j)_f\left(\alpha_f(\phi_{xi})_A + (1-\alpha_f)(\phi_{xi})_P\right)}{V_P\left(\alpha_f|\nabla\phi|_A + (1-\alpha_f)|\nabla\phi|_P\right)}$$

Delta function

$$\delta(\phi) = \frac{1}{2\alpha}\left(1 + \cos\left(\frac{\pi\phi}{\alpha}\right)\right) if |\phi| \le \alpha$$

$$\delta(\phi) = 0 if |\phi| \rangle 0$$

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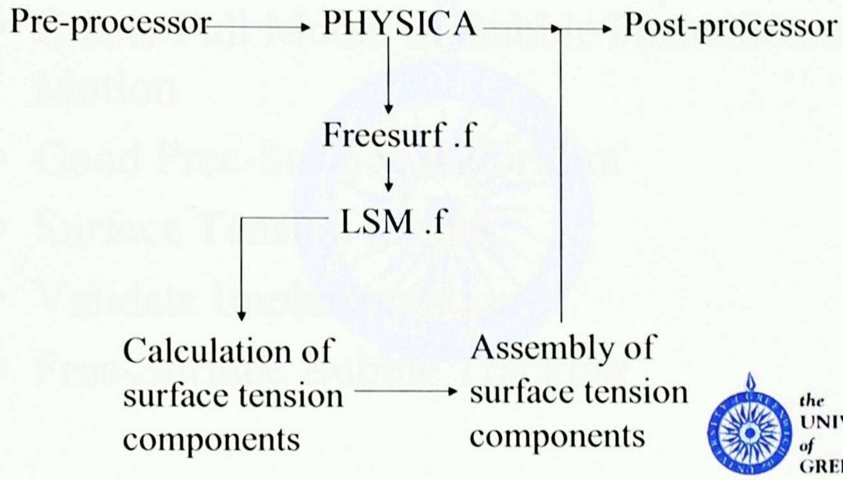
Level Set Method Implementation



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Accurate Surface Modelling

- Donor Acceptor — ☑ *Standard PHYSICA "SEA" algorithm*
- Van-Leer — ☑ *Implemented / Tested*
- C.I.P. method — ☑ *Coding nearly complete*
- V.O.F method — ☒ *Not used (similar to SEA)*

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Aims of Research

- Create Full Model of Bubble Formation and Motion
- Good Free-Surface Algorithm
- Surface Tension Model
- Validate Implementation
- Free-Surface Bubble Tracking

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Completed Work

- LSM Surface Tension implemented
- Tested With Various Cases
- LSM Surface Tension / Donor Acceptor Free Surface
- Tested With Collapsing Column and Complex Passage Cases
- Bubble Formation and Motion Modelled
- Tested With Various Cases

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Model Components

Mould Filling- Accurate Free Surface Model → Bubble Formation From Accurate Free-Surface Model → Switch to LSM / Van-Leer Surface Tension to Model Bubble → Track Bubble With Free-Surface Method / Lagrangian Particle Method

↓

FULL MODEL OF BUBBLE FORMATION / MOTION

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Results

- Surface Tension Model (Square to Circle)
- Accurate Free-Surface Model (Collapsing Column)
- Experimental Complex Passage*
- Rising Oil Bubble in Water (2 Phase Model)**
- Accurate Free-Surface Model Combined with Surface Tension Model (Collapsing Column with Bubble)
- Bubble Formation Modelled

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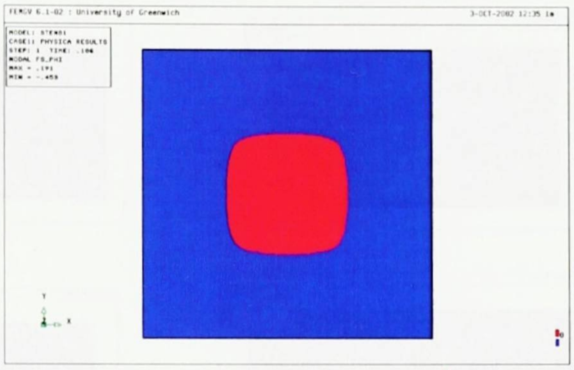
* Schmidt et al. MCWASP VIII, pp1131-1136, 1998

** Ref http://www.oslo.sintef.no/am/ns/research/movies/bubble.mpg

Square to Circle by Surface Tension

Mesh



Animation

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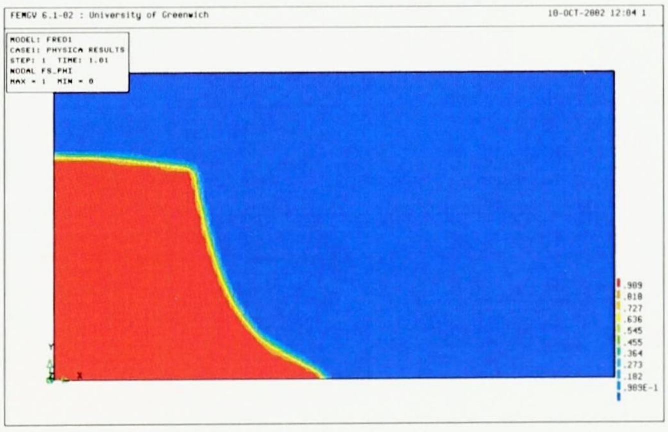
Collapsing Column with Donor Acceptor



Collapsing Liquid
Column 2D
Container
Properties of Water

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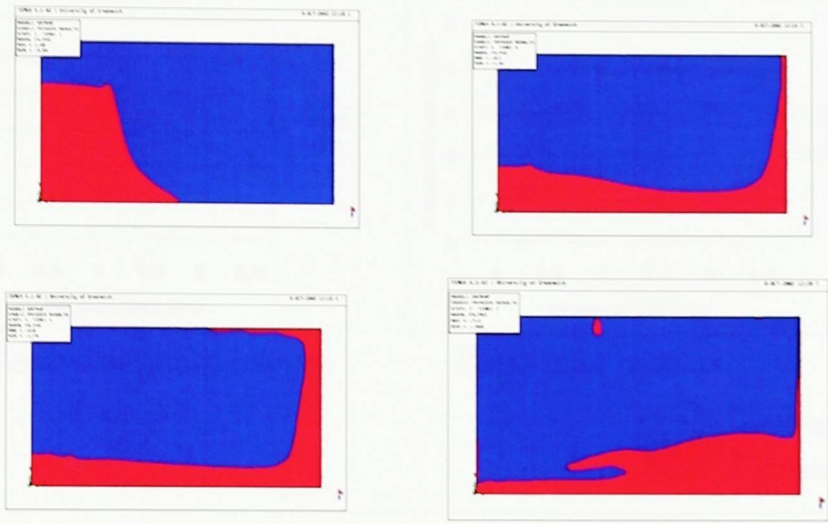
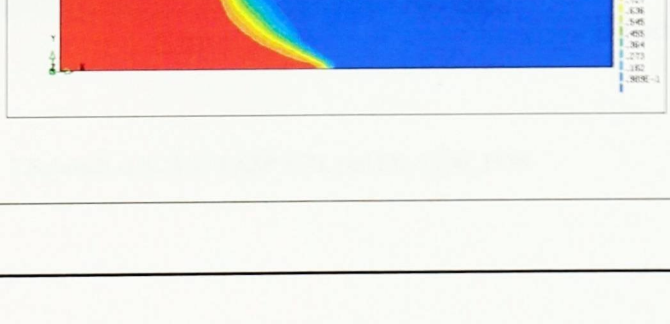
Time sequence: Donor-Acceptor



Collapsing Column with Van-Leer



Collapsing Liquid Column 2D Container Properties of Water

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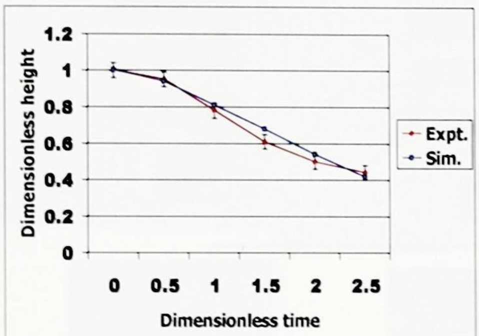
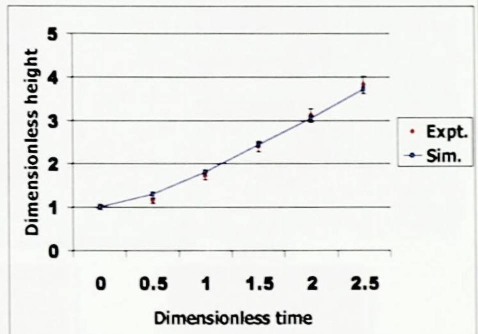
Simulation results & comparison

- Comparison with experiments performed by J. Martins and W. Moyce, 1952.



Vertical height of column.



Surge front position.

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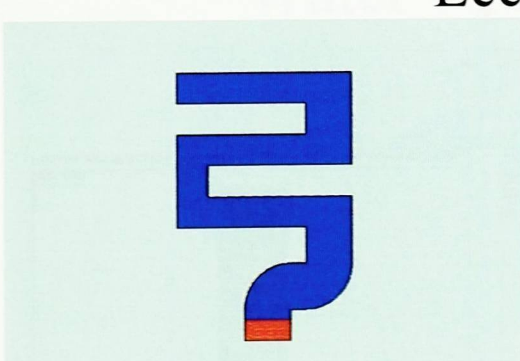
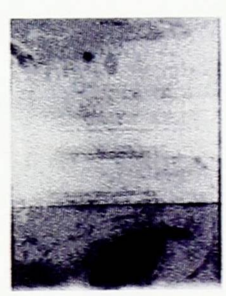
Filling of a Complex Passage – Van Leer



Simulation



Experiment *

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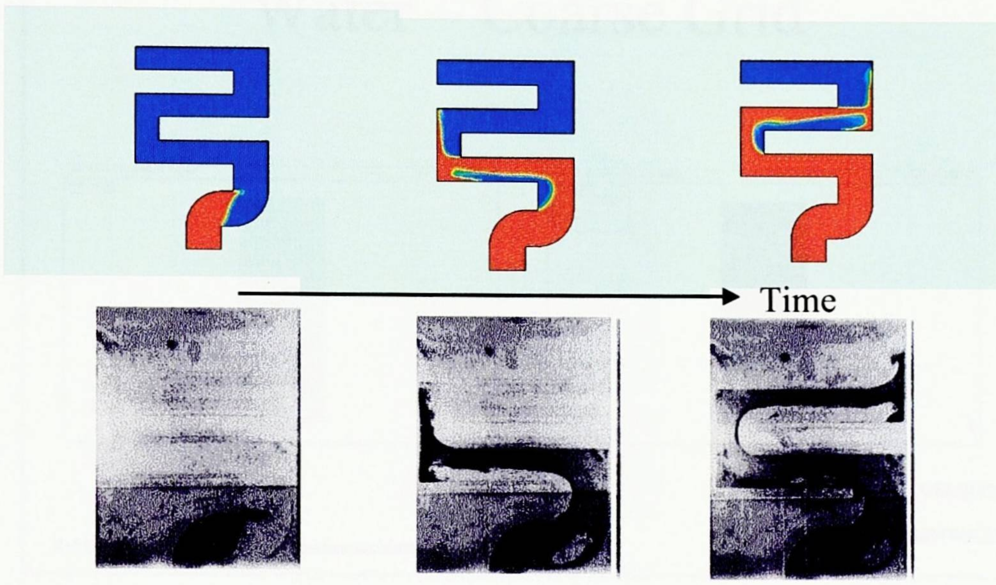
* Schmidt et al. MCWASP VIII, pp1131-1136, 1998

Comparison against experiment from [Schmidt, 1998]



Motion of Approx Oil Bubble in Water – Fine Grid

Ref http://www.oslo.sintef.no/am/ns/research/movies/bubble.mpg

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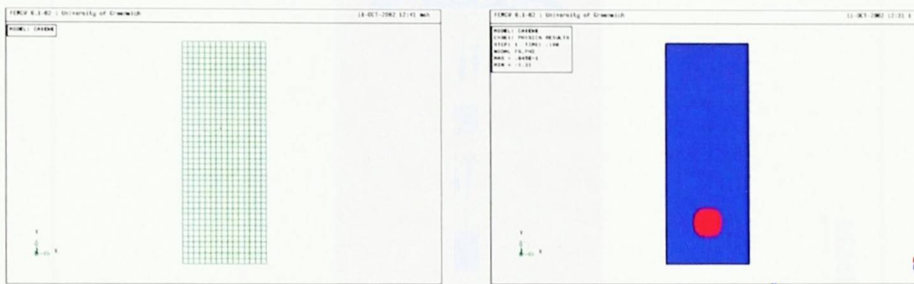
Motion of Approx Oil Bubble in Water – Coarse Grid



Ref:http://www.oslo.sintef.no/am/ns/research/movies/bubble.mpg

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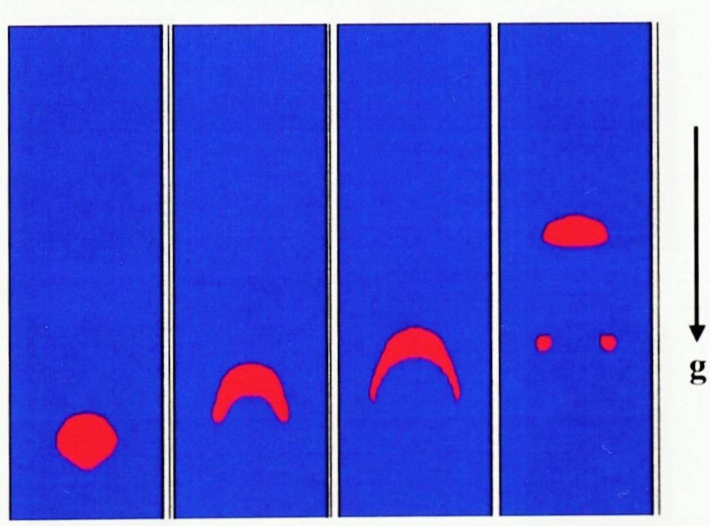
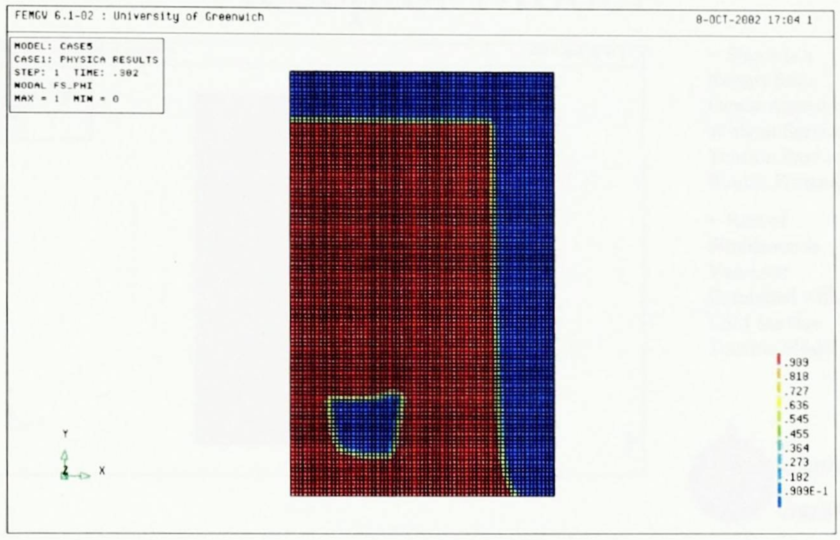
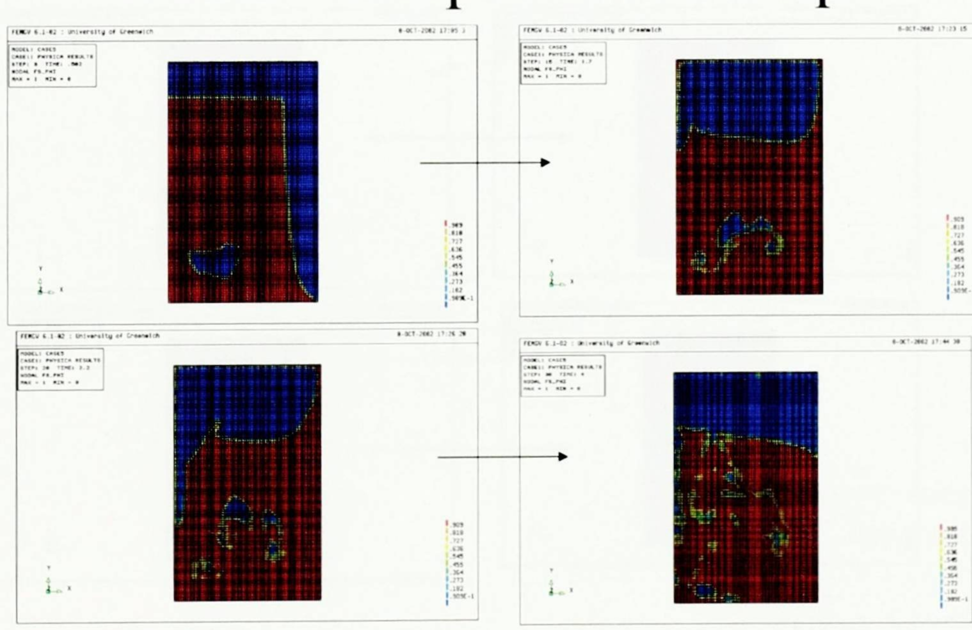
Rising bubble time sequence



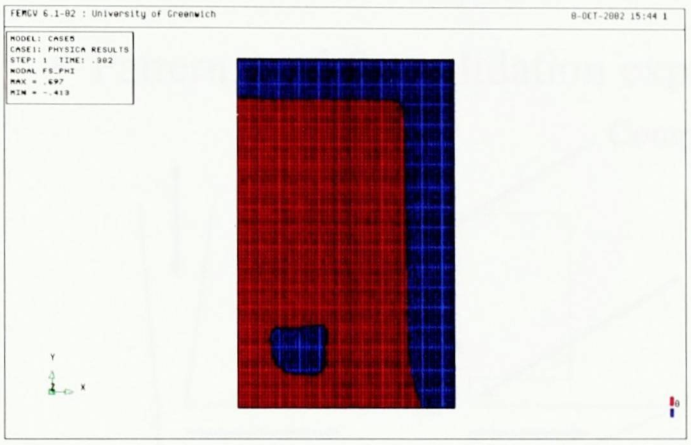
Free Surface -Donor Acceptor Model



Donor-Acceptor Time Seq.



Combined LSM and Donor Acceptor Model



- Step 1 is a Restart from Donor Acceptor Without Surface Tension Proving Bubble Formation
- Rest of Simulation is Van-Leer Combined with LSM Surface Tension Model

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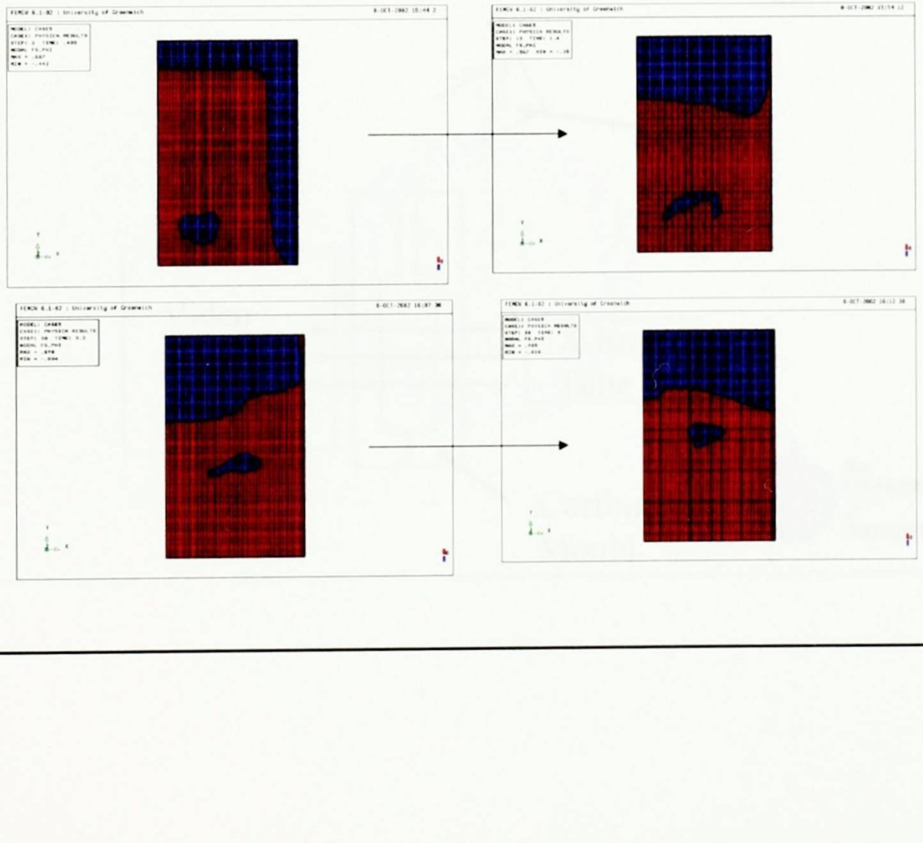
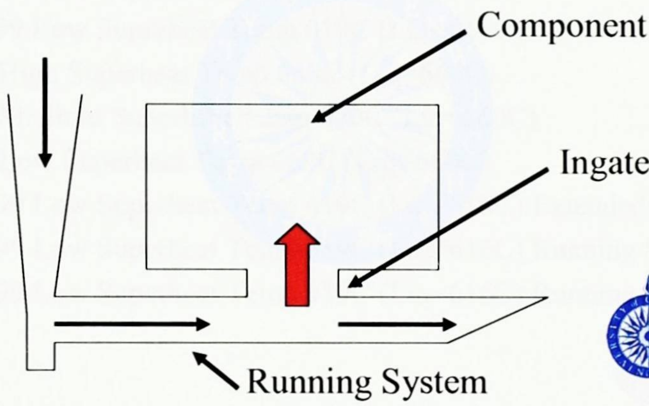
Hybrid LSM-Don.acc



Casting Mould

- Pattern used for validation experiments



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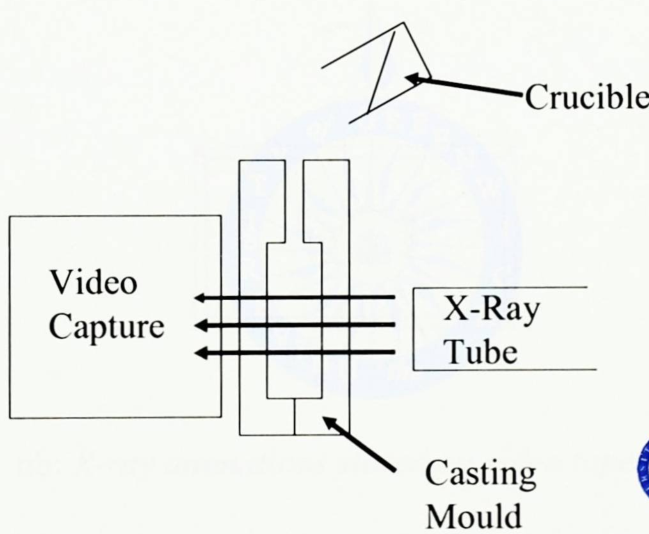
Real Time X-ray Footage



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Results

- 2L99 High Superheat Temp 635C (Liq=616C)
- 2L99 Medium Superheat Temp 625C (Liq=616C)
- 2L99 Low Superheat Temp 619C (Liq=616C)
- 2L99 Low Superheat Temp 619C (Liq=616C)
- 2L99 Low Superheat Temp 619C (Liq=616C)
- Al High Superheat Temp 680C (Liq=660C)
- Al Medium Superheat Temp 670C (Liq=660C)
- Al Low Superheat Temp 660C (Liq=660C)
- 2L99 Low Superheat Temp 619C (Liq=616C) Extended Down Sprue
- 2L99 Low Superheat Temp 619C (Liq=616C) Running Sys
- 2L99 Low Superheat Temp 619C (Liq=616C) Running Sys

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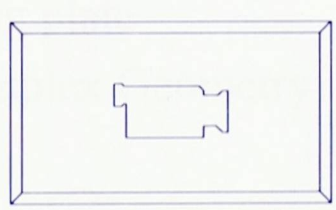
Real-Time x-ray results



nb: *X-ray animations stored on video tape shown here*

Conclusions

- LSM Satisfactory Model of Surface Tension
- Combined LSM/Donor Acceptor Model, Realistic Possibility of Predicting Bubbles In Casting
- Mesh Dependency is an Issue
- Criterion for Switching to Lagrangian tracking needed

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Remaining Tasks

- Compare with Experimental Data
- 3D Casting plate
- More Complex Geometry
- Write up

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