PHYSICA : A Multiphysics Computational Framework and its Application to Casting Simulations

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ABSTRACT

Metals casting is a process governed by the interaction of a range of physical phenomena. Most computational models of this process address only what are conventionally regarded as the primary phenomena - heat conduction and solidification. However, to predict other phenomena, such as porosity formation, requires modelling the interaction of the fluid flow, heat transfer, solidification and the development of stress-deformation in the solidified part of the casting. This paper will describe a modelling framework called PHYSICA[1] which has the capability to simulate such multiphysical phenomena.

1 INTRODUCTION

When a new casting design (i.e. part for a jet engine) is to be manufactured, the general practice of the foundry is to undertake numerous trials and tests to find the optimum design. This practice is obviously very expensive in man hours, materials and energy costs; in addition, it causes long lead times before production may commence. Until recently, the use of computational mechanics models to aid the foundry engineer has been negligible[2, 3]. This is primarily due to the complex nature of the process and the interacting physical phenomena present. During the casting process[4] a cold mould is filled with molten metal, which cools and solidifies. As the cooling progresses thermal gradients build up in the metal. In the liquid regions this promotes thermal convection that redistributes heat around the casting. Before the onset of solidification the casting is in full contact with the surrounding mould, but as the casting solidifies it begins to pull away from the mould, developing a gap. This gap restricts the flow of heat from the metal to the mould, hence influencing the manner in which the cast component solidifies. To simulate such a process the computational modeller must address the following;

- Fluid flow analysis of mould filling.
- Thermal convection once the mould has filled.
- Thermal analysis of solidification and evolution of latent heat.
- Deformation and residual stress predictions of solidified component.
- Porosity formation.

Discretisation methods used in computational mechanics have historically followed two distinct routes. Finite Element (FE) methods have generally been adopted for discretising the solid mechanics equations and Finite Volume (FV) methods have been used for the conservation equations governing fluid flow. However, during the last few years FV methods have also been employed to analyse solid mechanics problems on unstructured meshes[5, 6, 7]. Such methods have proved to be as accurate as finite elements in analysing both linear and nonlinear materials.

For multiphysical processes, such as metal casting, a unified computational framework is required to couple the numerous physical phenomena.

2 A MULTIPHYSICS ENVIRONMENT

A common element in all computational mechanics codes is the mesh representing the domain. Various methods can be used to discretise the governing equations over the mesh. For FV procedures the evaluation of fluxes across cell/element faces, volume sources and coefficients of the linear solvers are generic, being essentially based on mesh geometry and materials properties within a cell. PHYSICA is a software framework which has generic tools that concentrate on objects (i.e mesh faces, etc.) and their relations in evaluating all the relevant terms (diffusion, convection, source, etc.) at a generic level. Figure 1 shows the design principles inherent within the PHYSICA framework and Figure 2 shows the various levels of abstraction. It is expected that the majority of modellers would only use the top three levels. So, for example a new higher order convection scheme may be inserted by the user at the 'Algorithm' level and the modular structure of the code will allow compatibility with all other routines. Such a computational framework reduces model development times. At present PHYSICA has the following capabilities;

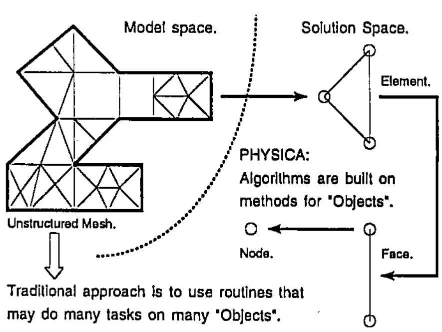

Figure 1: PHYSICA - Design principles.

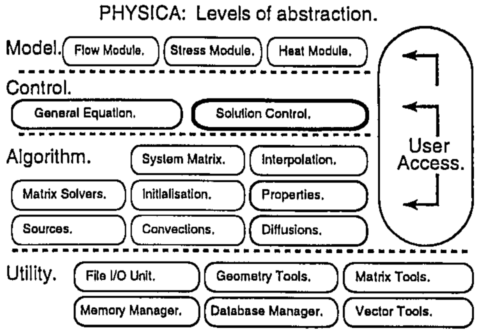

Figure 2: PHYSICA - Level of code abstraction.

- Data structures for vertex-based tetrahedral, pentahedral, hexahedral and cell centred polyhedral elements.
- SIMPLE based algorithms for incompressible Navier Stokes Equations.
- Free surface flow algorithm.
- Range of turbulence models.
- Source based solidification/melting procedures.
- Elasto-visco-plastic solid mechanics algorithm.
- Solvers which include CG, BiCG, SOR and Jacobi.
- Hooks to pre and post-processing packages.

PHYSICA is currently being used to simulate a number of multiphysical processes, which includes metals casting.

3 GOVERNING EQUATIONS

The equations that represent the governing physics of heat transfer, fluid flow and solid mechanics in three-dimensional space are:-

3.1 Computational Fluid Dynamics (CFD)

The general equations that govern three-dimensional transient fluid flow are given by the momentum and mass continuity equations which are stated in their vector form below,

$$\frac{\partial}{\partial t}(\rho\underline{u})+\nabla.(\rho\underline{u}\underline{u}) = \nabla.(\mu\nabla\underline{u})-\nabla p+\underline{S}, \quad (1)$$

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho\underline{u}) = 0, \quad (2)$$

where $\underline{u}$ is the velocity vector. The other variables at time t are ρ, the material density, μ, the dynamic viscosity, and the pressure p. The source term $\underline{S}$ in equation(1) contains the buoyancy and Darcy terms due to temperature changes and solidification.

Heat transfer is governed by the energy equation,

$$\frac{\partial(\rho h)}{\partial t} + \nabla.(\rho\underline{u}h) = \nabla.(k\nabla T) + S_h, \quad (3)$$

where h, k and T are the enthalpy, thermal conductivity and temperature respectively. The evolution of latent heat is included in the source term

$$S_h = \frac{\partial(L\rho f_l)}{\partial t} - \nabla.(L\rho\underline{u}f_l), \quad (4)$$

where L and f_l are the latent heat and liquid fraction respectively.

3.2 Computational Solid Mechanics (CSM)

In tensor form, the incremental equilibrium equations are

$$\Delta\sigma_{ij,j} = 0, \quad (5)$$

where the incremental stress is related to the incremental elastic strain via Hooke's law;

$$\{\Delta\sigma\} = [D]\{\Delta\epsilon_e\}, \quad (6)$$

where [D] is the elasticity matrix. For the deformation of metals, the von-Mises yield criterion is employed and the incremental elastic strain is given by

$$\{\Delta\epsilon_e\} = \{\Delta\epsilon\} - \{\Delta\epsilon_t\} - \{\Delta\epsilon_{vp}\}, \quad (7)$$

where $\{\Delta\epsilon\}$, $\{\Delta\epsilon_t\}$ and $\{\Delta\epsilon_{vp}\}$ are the total, thermal and visco-plastic incremental strain, respectively. The visco-plastic strain rate is given by the Perzyna[8] model

$$\frac{d}{dt}\{\epsilon_{vp}\} = \gamma\left\langle\frac{\sigma_{eq}}{\sigma_y} - 1\right\rangle^{\frac{1}{N}} \frac{3}{2\sigma_{eq}}\{s\}, \quad (8)$$

where σ_{eq}, σ_y, γ, N and s are the equivalent stress, yield stress, fluidity, strain rate sensitivity parameter and deviatoric stress, respectively. The $<.>$ operator is defined as follows:

$$<.>=\begin{cases} 0 & \text{when} \quad . \leq 0 \\ . & \text{when} \quad . > 0 \end{cases} \quad (9)$$

The incremental total strain for infinitesimal strains is

$$\{\Delta\epsilon\} = [L]\{\Delta d\}, \quad (10)$$

where [L] is the differential operator matrix and $\{\Delta d\}$ is the incremental displacement.

4 DISCRETISATION

All of the above equations are discretised on unstructured meshes using FV procedures. For the CFD equations the control volumes are cell-centred[9, 10], and for the CSM equations, the control volumes are vertex-based[11]. It should be noted that the same mesh is used to represent the domain in question and generate the control volumes. The dependent variables resulting from the discretisation are fluid velocities, enthalpy and solid displacement increments. The resulting system of discretised equations are of the form

$$[A]\{\Phi\} = \{b\}, \quad (11)$$

where [A] is the system matrix and {b} contains source terms for the dependent variables $\{\Phi\}$ which are velocities, enthalpy and displacement increments.

5 SOLUTION PROCEDURE

The complete solution procedure for solving the coupled fluid and solid mechanics equations in metals casting is:-

1. Solve momentum and continuity equations.
2. Solve energy equation.
3. Evaluate other variable quantities, eg. material properties, etc..
4. Repeat steps 1-3 until convergence.
5. Solve CSM equations.
6. Update total stress variables.
7. Recalculate geometrical quantities.
8. Repeat steps 1-7 for time-step advancement.

Note, in step 7, the geometrical quantities are recalculated due to the changes in displacement from the CSM analysis, and the equations in steps 1 and 2 rediscretised over the updated mesh.

5.1 Boundary Conditions

It is important when predicting how a cast shape develops to be able to model the thermal changes correctly. Consequently, account must be taken of the gap formation at the mould/cast interface. For this analysis coincident nodes have been used to model the interface. This enables the cast component to move freely away from the mould. The boundary condition at this interface is given by

$$\frac{\partial T}{\partial n} = h_{eff}(T_c - T_m), \qquad (12)$$

where T_c, T_m and h_{eff} are the cast temperature, mould temperature and effective heat transfer coefficient which is given by

$$h_{eff} = \frac{k_{gap}}{d_{gap}}, \qquad (13)$$

where k_{gap} and d_{gap} are thermal conductivity of the gap medium and the gap distance. During the analysis the mould is assumed to be rigid and hence the mechanical contact analysis is reasonably straight forward.

6 RESULTS

The following results will show two test cases that illustrate the complexity involved in modelling the multiphysical phenomena present in the the casting process. The simulations will both assume an initial fill state and start with a uniform temperature in the molten metal and mould.

The first test case compares numerical predictions with experimental results[12] for the die casting of a hollow aluminium cylinder. Figure 3 shows the experimental design where the top and bottom of the component are insulated to ensure a one dimensional heat loss to the mould material. Thermocouples were inserted into the

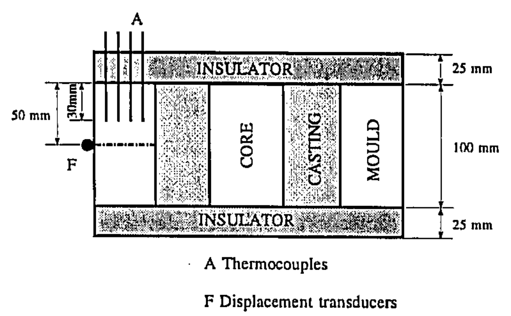

Figure 3: Experimental design of cylinder casting (side View).

mould and a displacement transducer attached to the cast component to monitor the gap formation at the cast/mould interface. A fully coupled analysis was undertaken in PHYSICA to simulate the solidification and resulting solid deformation of this component. The materials properties of the steel mould and core and aluminium casting are given in Tables 1, 2 and 3 (see Appendix). The heat transfer coefficient

h_{eff} was assumed to vary linearly between $400W/m^2K$ to $20W/m^2K$ corresponding to gap distances of 0.0mm to 0.5mm.

Figure 4 illustrates the predited deformation of the cast cylinder over time. As expected, this contracts away from its surrounding mould and into the internal core, leaving gaps at the top and side interfaces.

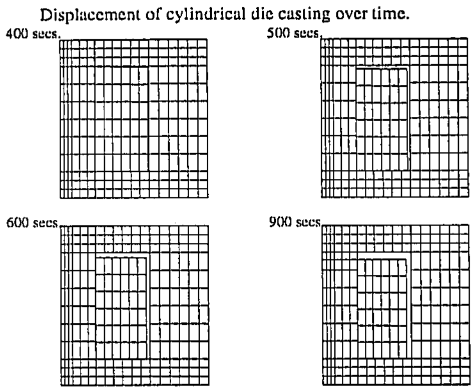

Figure 4: Gap formation over time (x10).

Figue 5 compares predicted temperatures, with and without gap formation, for both the cast and mould against gathered experimental readings. The top curves show temperatures for a location in the casting. Including mechanical effects in the simulation, i.e gap formation, results in a closer prediction to experimental data. The bottom curves show similar results for a location in the mould. In summary, neglecting the formation of an air gap at the cast-mould interface will affect the the rate at which heat is lost, and possibly the manner in which the casting solidifies.

Figure 6 shows the resulting gap formation at the vertical cast/mould interface over time, where the insulation is allowing uniform contraction across the casting. It can be seen that the predictions compare well with the experimental data.

The next test case shows the stress and porosity distributions in a three dimensional casting. In this simulation, fluid flow, solidification and deformation are fully coupled. Figure 7 illustrates the amount of thermal convection in the initial stages of cooling.

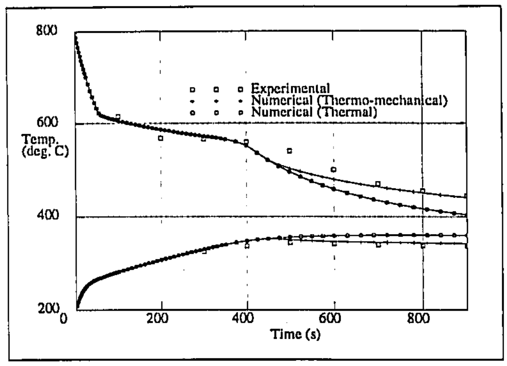

Figure 5: Temperature profiles in casting and mould.

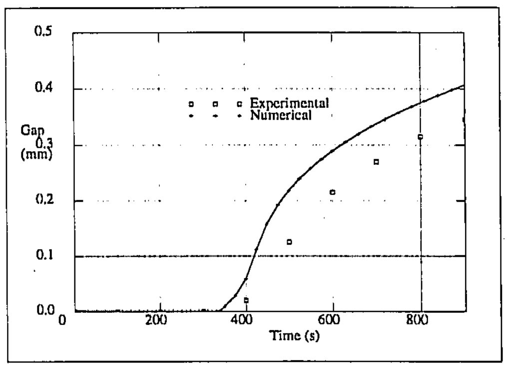

Figure 6: Evolution of gap at cast/mould interface.

It is interesting to note the large flow rates

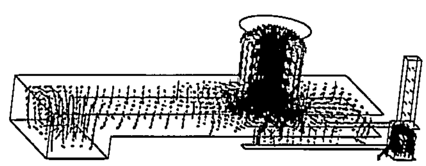

Figure 7: Thermal convection in 3D casting.

from the feeder (i.e the cylinder) to other parts of the casting. This is what is to be expected as an insulating material has been placed around the feeder to ensure that it remains in a liquid state and can feed areas of the casting which are prone to shrinkage porosity. Figure 8 shows the resulting von-Mises stress distribution across this casting where the large magnitudes of stress are located at the centre of the plate between the step and the feeder. This is also expected

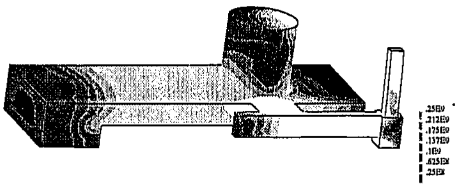

Figure 8: Final residual stress profile in casting.

as the current design restricts contraction in this area due to the casting geometry. Figure 9 shows a cross section of the casting and its von-mises stress profile. The final deformed shape can clearly be seen with large gaps appearing at aither end of the casting. The effect of convection in the cast component on the final cooling profile was also investigated. Figure 10 shows the differences in cooling curves for analyses with and without convection (note, the top curve represent the cast and lower curve the mould). Differences of up to approximately 50°C can be observed, where thermal convection in the cast metal allows redistribution of heat from hotter areas to cooler areas near the interface, thus resulting in faster cooling. Figure 11 shows the porosity predictions using the Niyama criteria[13]. This empirical rule is equal tothe local thermal gradient divided by the square root of the local cooling rate. If this value is less than unity then thier is a high liklihood of porosity occuring. Figure 11 shows the contours where this value is equal to one. These predictions seem feasible as the simulations predicted that the feed path from the feeder(i.e the cylinder on top of the plate) to the step region of the casting is cut off before the step region completely solidifies.

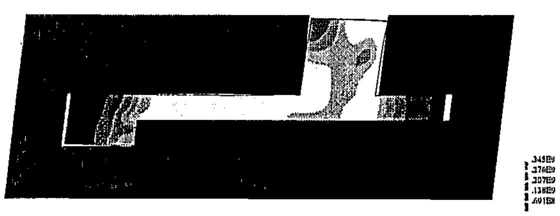

Figure 9: Gaps at cast/mould interface.

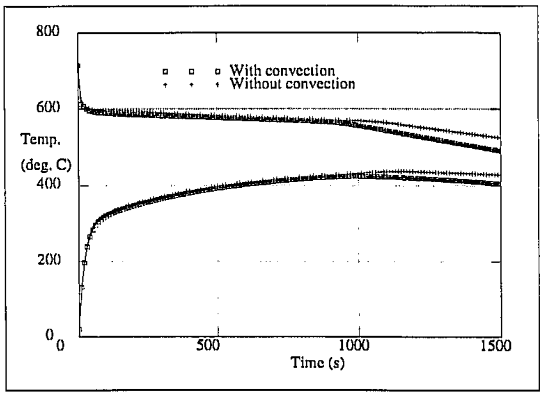

Figure 10: Cooling curves in mould and cast component.

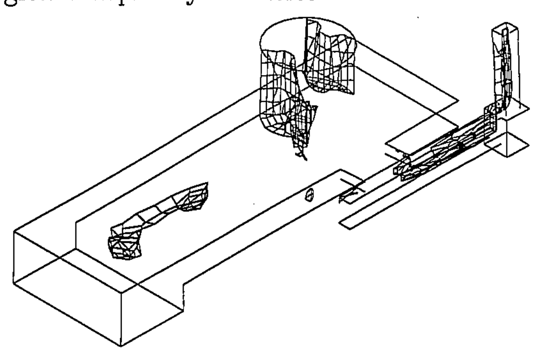

Figure 11: Porosity predictions using Niyama.

7 CONCLUSIONS

Increasingly, there is a requirement in engineering processes to model multiphysical phenomena. The rationale behind the PHYSICA framework is to supply modellers with a tool which allows ease in developing computational based models, where coupling between complex multiphysical phenomena can be accomplished in a robust and efficient manner. Metals casting is an example of such a process that involves fluid flow, heat transfer, solidification and solid mechanics. This paper has presented results of two casting simulations. Comparisons between predicted and available experimental data are encouraging.

Currently, the functionality of the computational FV framework PHYSICA is being extended to include models for magneto-hydro-dynamics, radiation, macro- and micro- porosity and combustion.

ACKNOWLEDGEMENTS

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References

[1] PHYSICA, University of Greenwich, London, UK. Email physica@gre.ac.uk

[2] M. Cross and J. Campbell,"Modeling of Casting, Welding and Advanced Solidification Processes VII", published by the Materials, Metals and Minerals Society, Warrendale, PA, (1995)

[3] C. Bailey, P. Chow, M. Cross, Y. Fryer and K. Pericleous, " Multiphysics modelling of the metals casting process.", Proc. R. Soc. Lond. A, **452**, pp 459-486, (1996).

[4] J. Campbell, *Castings*, (Butterworth-Heinemann, Oxford, (1991).

[5] E. Onate, M. Cervera and O. C. Zienkiewicz, "A finite volume format for stuctural mechanics", Int. Journal for Num. Methods in Engg, 37, 181-201 (1994).

[6] C. Bailey, M. Cross, A finite volume format for structural mechanics. Int. Jnl Num Methods Engg. **10**, 1757-1776, (1995).

[7] G. Taylor, C. Bailey and M.Cross, "Solution of elastic/viscoplastic constitutive equations : A finite volume approach" Appl. Math Modelling, 19, 746-760, (1995)

[8] P. Perzyna, "Fundamental problems in viscoplasticity", Advan. Appl Mech, 9, 243-377, (1966)

[9] P. Chow, M. Cross, An enthalpy control volume unstructured mesh (CV-UM) algorithm for solidification by conduction only. Int. Jnl Num Methods Engg. **35** (1992), 1849-1870.

[10] P. Chow, Control Volume Unstructured Mesh Procedure for Convection-Diffusion Solidification Processes. PhD thesis, University of Greenwich, (1993).

[11] G. Taylor, A Vertex Based Discretisation Scheme Applied to Material Non-Linearity within a Multiphysics Finite Volume Framework, Ph.D Thesis, University of Greenwich (1996).

[12] P. Schmidt, I Svensson, Heat transfer and air gap formation in permanent mould casting of aluminium alloys, Technical report TRITA-MAC-0541, Materials research centre, Royal Institute of Technology, Stockholm, 1994.

[13] E. Niyama, T. Uchida, M. Morikawa, S. Saito, "Method of shrinkage prediction and its application to steel castings practice". AFS casting metals research journal. (1982), 52–63.

APPENDIX

T_L	Liquidus temperature	618.8°C	
T_S	Solidus temperature	566.4°C	
h	Latent heat of fusion	440 kJ/kg	
k	Thermal conductivity	150 W/(mK)	
ρ	Density	2,710 kg/m^3	
c	Specific heat capacity	1,160 J/(kgK)	
α	Coefficient of thermal expansion	5×10^{-5} /K	
ν	Poisson's ratio	0.33	
E	Young's modulus	60,000MPa	20°C
		34,000MPa	450°C
		1×10^{-2}MPa	566.4°C
Y	Yield stress	500MPa	20°C
		1×10^{-4}MPa	566.4°C

Table 1: Material properties of the aluminium casting alloy.

k	Thermal conductivity	33 W/(mK)
ρ	Density	7,880 kg/m^3
c	Specific heat capacity	600 J/(kgK)

Table 2: Material properties for the steel mould material.

k	Thermal conductivity	0.1 W/(mK)
ρ	Density	1,000 kg/m^3
c	Specific heat capacity	1,760 J/(kgK)

Table 3: Material properties for the insulation.