Simulation of Core Gas Production During Mold Fill

P. Scarber, Jr. The University of Alabama at Birmingham

C.E. Bates The University of Alabama at Birmingham

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ABSTRACT

Subsurface porosity, oxides, and entrained gas produce some of the most aggravating defects encountered in the production of aluminum castings. These defects are difficult to control and may not be found until castings are cleaned, machined and inspected. Gases evolved during mold filling may float through the casting and leave oxide trails and subsurface cavities.

Simulations of mold fill and solidification have increased in accuracy over the past few decades and can now model the formation of many commonly observed casting anomalies, such as shrinkage, reoxidation, and cold metal defects. However, there has not been much emphasis on simulating the formation and movement of core gas during mold fill.

A subroutine was developed to simulate the formation of core gas that forms during binder pyrolysis in silica sand cores bonded with phenolic urethane. This simulation was a single phase model, so core gas was not allowed to bubble through liquid metal. The subroutine used data gathered by the UAB Core Gas Consortium as input for the core gas generation.

Total gas volumes and gas evolution rates for cores immersed in liquid iron and liquid aluminum were in reasonable agreement between simulations and experimental observations. The rate curves for the simulation were shifted in time relative to the experimental curves, which was probably due to improper selection of heat transfer coefficient values in the simulations. However, the core gas subroutine was fairly accurate using the simplified physical model presented in the paper.

INTRODUCTION

Pores associated with gas from cores, molds, binders and additives can be difficult to detect, and they are often not found until castings are cleaned, machined and inspected. A subsurface pore in an aluminum head casting located just above a water jacket core, is illustrated in Figure 1. This pore was found when the casting was drilled and tapped. A subsurface blow in a casting with a solid core is illustrated in Figure 2.



Figure 1. (A) Porosity and (B) Oxide Trail in Aluminum Head Casting Above the Water Jacket Core.



Figure 2. Subsurface Gas Defect in a casting with a solid core.

Computer programs have been developed to predict metal flow to minimize turbulence, but there is much to learn about bubbles, folds, oxides, and pores produced by mold and core gases during pouring. Foundries have historically used their experience to design mold and core packages and then they "pour and pray". There is relatively little data to help select a binder, coating, or core vent geometry to predict or eliminate gas porosity.

The focus of this paper is to present the pertinent factors for simulation of core gas produced from binder pyrolysis during mold fill and illustrate simulation results. The experimental data used in the simulations, as well as the physical model for core gas generation, were gathered from the Core Gas Consortium, hosted by the University of Alabama at Birmingham.

A subroutine for predicting the generation and movement of core gas was developed and compared with experimental findings for silica sand cores bonded with 1.5% phenolic urethane binder and immersed in liquid aluminum or liquid iron. The subroutine was written to work in conjunction with the general fluid dynamics code Flow-3D, produced by FlowScience, Inc.

THEORY

Surface and sub-surface gas porosity causes a significant amount of scrap in the casting industry. In general, gas porosity can originate inside or outside the metal being poured. Exogenous sources include air initially in the mold cavity that was entrained during pouring, hydrogen and other gases produced by metal-mold reactions, reactions of metal with chaplets, and gases emitted by cores and coatings. (Portevin, 1952)

Endogenous sources of porosity include those formed by precipitation of dissolved gas and those formed by chemical reactions, such as hydrogen formed between liquid metal and moisture in the mold or air, as described in the following equation for aluminum:

$$2Al + 3H_2O \rightarrow Al_2O_3 + 3[H]$$
 Equation 1

Binder pyrolysis can inject gas into the metal, and the gas is usually entrapped near the cope surface or under cores. Since gas bubbles may float some distance before becoming entrapped, identifying the source is sometimes difficult. (Worman, 1973)

Gases may not be trapped if they are evolved while the metal is completely liquid, but they can damage the casting by leaving an oxide trail, dross or dissolved gas. (Caine, 1966 and Campbell, 1997) Each of these factors was evaluated in order to develop a physically meaningful simulation of core gas generation and movement.

To simulate core gas, it is necessary to understand the mathematical description of fluid motion. The movement of an incompressible Newtonian fluid through a fixed volume in space over a small period of time is governed by a mass balance equation as follows:

$$\frac{V_F}{\rho c^2} \frac{\partial p}{\partial t} + \frac{\partial u A_x}{\partial x} + \frac{\partial v A_y}{\partial y} + \frac{\partial w A_z}{\partial z} = \frac{RSOR}{\rho}$$
Equation 2

where V_F is the fractional volume open to flow; ρ is the fluid density; c is the speed of sound in the liquid; p is the pressure; u, v, and w are the component velocities in each of the cardinal directions; A_x , A_y , and A_z are the areas open to flow in each of the cardinal directions; and RSOR is a density source with no momentum. (FlowScience, Inc., 2004) The mass balance equation must be solved simultaneously with the Navier-Stokes equations of momentum in order to fully describe the liquid being simulated:

$$\frac{\partial u}{\partial t} + \frac{1}{V_F} \left(uA_x \frac{\partial u}{\partial x} + vA_y \frac{\partial u}{\partial y} + wA_z \frac{\partial u}{\partial z} \right) = G_x + f_x - \frac{1}{\rho} \frac{\partial p}{\partial x} - b_x - \frac{RSOR}{\rho V_F} u$$
 Equation 3

where G_x is a body acceleration, f_x is viscous acceleration, and b_x is flow loss through porous media. (FlowScience, Inc., 2004) There is a similar equation for momentum in the y- and z-directions as well.

The term for flow losses in porous media is of particular importance for the movement of gas in cores and molds. The coefficient of drag associated with flow through a porous compact of granular material is proportional to the square of fluid velocity and can be summarized as follows:

$$K = \frac{\mu}{\rho} \frac{1 - V_F}{V_F} \left(a_0 \frac{1 - V_F}{V_F} + b_0 \frac{Re}{d} \right)$$
 Equation 4

where a_0 and b_0 are related to the Non-Darcian flow coefficients, d is the average particle diameter, and Re is the Reynolds number. Gas created within a porous obstacle would be generated at a rate given by the user, RSOR, as shown in the mass conservation and momentum equations shown in Equations 2 and 3.

Binder pyrolysis was assumed to begin at a specific temperature in the core gas simulations in order to simplify the gas generation physics. Obstacle temperatures were governed by the general heat flow equation:

$$(1 - V_F) \rho_w C_w \frac{\partial T_w}{\partial t} - \frac{\partial}{\partial x} \left[k_w (1 - A_x) \frac{\partial T}{\partial x} \right] - \frac{\partial}{\partial y} \left[k_w (1 - A_y) \frac{\partial T}{\partial y} \right] - \frac{\partial}{\partial z} \left[k_w (1 - A_z) \frac{\partial T}{\partial z} \right] = TSOR \quad Equation 5$$

where ρ_w , C_w , k_w , and T_w are solid material values for density, specific heat capacity, thermal conductivity, and temperature, respectively, and TSOR is an energy source term due to liquid-solid heat transfer and external heat sources (FlowScience, Inc., 2004) TSOR would also include all heat energy input from phase transformations and radiative heat transfer from the liquid.

Flow-3D, produced by FlowScience, Inc., was modified in such a way as to allow generation of a fluid from within a simulated obstacle using the RSOR term in the mass balance equation above (Equation 2). Each computational cell within an obstacle that contains a certain amount of binder would produce gas at a certain rate once a certain temperature was reached, both of which would be provided by the user. The user would also have to input the total gas volume generated per mass of bonded material, which can be determined from either thermo-gravimetric analysis (TGA) data or loss-on-ignition (LOI) tests. Gas evolution would continue until the specified maximum gas volume is reached, at which time the computational cell would stop producing gas but still allow gas to pass through it. The user input necessary for the subroutine is shown in Table 1; the data input listed in the table would be accompanied by other input necessary to run a thermal simulation, such as bonded material density and specific heat.

Preprocessor Input Required for Core Gas Simulation	
Volume of Gas per Mass of Bonded Material	
Binder Vaporization Temperature	
Time for Binder Vaporization	

 Table 1.
 User Input Variables for Core Gas Simulation.

EXPERIMENTAL PROCEDURES

The experimental data used for comparison to the simulation results was collected by the UAB Core Gas Consortium. Sand cores were commercially prepared as solid cylinders with a diameter of 1.125 inches by 8 inches long. Two inch long specimens were cut from these cores and immersed in either molten A 356 aluminum or molten gray iron and the rates of gas evolution were determined. Sand permeability was measured using procedures previously published. (Winardi, 2005)

A schematic of the core immersion apparatus is illustrated in Figure 3. The hot gases formed from binder pyrolysis during aluminum contact flowed through a preheated line (to minimize condensation) and displaced oil in a preheated chamber. The displaced oil flowed from the chamber into a container placed on a precision electronic balance, and the weight of displaced oil was measured as a function of time. From the oil weight and density, the volume of gas was calculated. Temperatures were also measured at several points to be sure the piping and oil chamber were hot enough to prevent water condensation. The precipitation of one gram of water in the system represents a loss of 1 liter of gas volume.



gas evolution volume and rate for sand cores.

In the simulations, the only fluid considered was the gas generated as a result of binder pyrolysis. The molten metal was approximated by an obstacle with the density, specific heat capacity, and thermal conductivity of either molten aluminum or iron. The thermal properties of the core sand were obtained from data published by Midea and Shah for fine sand bonded with phenolic urethane. (Midea, 2002) The core gas input data was obtained from the Core Gas consortium for core sand bonded with 1.5% phenolic urethane and no additives.



Figure 4. Temperature distribution in the core, core holder, and molten metal bath at time=0 in the simulation.

Figure 4 shows the temperature distribution in the simulation at time=0. Both the core and core holder were set at an initial temperature of 25 °C and the liquid metal, which was aluminum in this case shown in the figure, was set at 627 °C. No heat transfer was assumed to occur between the core holder and the liquid metal since experimental tests included an insulating sleeve around the core holder.

RESULTS AND DISCUSSION

Figure 5 shows fluid temperature contour plots during the first stages of immersion in liquid aluminum at 627 °C. Gas is generated at the surface of the core almost instantaneously as shown in 5(a), which would be expected since this area would experience extremely fast heating. The generated gas moves inward into the core, shown in 5(b), and then is pushed out of the core as shown in 5(c) and 5(d). An interesting observation is the rapid cooling of the core gas as it moves through the core. The gas is generated at the surface and is initially relatively hot, but quickly cools to below 327 °C as it moves through the cool interior of the core. The rapid cooling of the core gas in the simulation means that high density pyrolysis products could recondense within the core – a phenomenon that often occurs in green sand castings. (Marek, 1963 and Draper, 1969)

Figure 6 shows a plot of evolved gas volume and gas evolution rate vs. time of a silica sand core containing 1.5% phenolic urethane binder immersed in liquid aluminum. The rate curve for the simulation shows irregular behavior in the initial seconds of immersion, due to the relatively low heating rate in this time frame. In the first seconds of the simulation, only a small number of elements have reached the temperature required to evaporate the binder. After 6 or 8 seconds, a much larger volume of material is at or above the binder pyrolysis temperature, which accelerates the gas evolution rate in the simulation.

The total generated gas volume in the simulations is in reasonably good agreement with experimental measurements. The shape of the volume curve for the simulation is not completely similar to that for the experimental measurements, but this may be due to improper selection of heat transfer coefficient between the liquid metal and sand core in the simulations. The rate curve for the simulation shows two distinct humps, similar to the behavior seen in experimental tests, except that the simulation humps occur at a later time than in experiments. Again, this difference may be due to an incorrect heat transfer coefficient in the simulations.

Figure 7 shows a plot of evolved gas volume and gas evolution rate vs. time of a silica sand core containing 1.5% phenolic urethane binder immersed in liquid iron at 1343 °C. Just as was the case for aluminum immersion, the humps in the rate curve from the simulation occur at a different time than the experimental rate curve. The total gas volume curves for the simulation and experiment were relatively similar, but the simulation produced much more gas than the experimental cores in the first 30 seconds. This difference could be due to an incorrect heat transfer coefficient or an over-estimation of the total gas volume per gram of bonded material which was used as input for the core gas subroutine. However, the results from these first simulations were within 15% accuracy of the experimental observations, proving the validity of the assumptions made in this first stage of core gas simulation.



Figure 5. Fluid temperature contours for a silica sand core with 1.5% phenolic urethane binder immersed in liquid aluminum at 627 °C after (a) 0.29 s, (b) 0.56 s, (c) 0.79 s, and (d) 1.8 s.



Figure 6. Plot of total evolved gas volume and gas evolution rate vs. time for a silica sand core containing 1.5% phenolic urethane binder immersed in liquid aluminum at 627 °C.



Figure 7. Plot of total evolved gas volume and gas evolution rate vs. time for a silica sand core containing 1.5% phenolic urethane binder immersed in liquid iron at 1343 °C.

CONCLUSIONS

A subroutine was developed to simulate the generation of gas as a result of binder pyrolysis within a bonded sand core during immersion in liquid aluminum and liquid iron. The simulation used the total gas volume generated per mass of bonded material, the pyrolysis temperature, and the pyrolysis time as input to the core gas subroutine. The simulation was a single phase flow model – only the generated core gas was simulated.

The simulations showed similar behavior in total gas volume and gas evolution rate to the experimental observations for core immersion in both liquid iron and liquid aluminum. Future simulation work will focus on more accurate heat transfer coefficient data, which should increase the simulation accuracy.

This simulation work is intended to assist aluminum and iron foundries in minimizing gas defects in castings by accurately simulating the formation of core gas related defects.

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