FINAL TECHNICAL REPORT

Development of a Computational Fluid Dynamics (CFD) Software Package To Support the Engineering of Lost Foam Pattern

Blowing and Steaming:

Arena-flow-eps

February 2003

FINAL TECHNICAL REPORT:

Development of a Computational Fluid Dynamics (CFD) Tool for Modeling the Blowing and Steaming of Expandable Polystyrene Patterns for Lost Foam Casting: *Arena-flow-eps*

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Project Objective: Develop a new CFD software tool (*Arena-flow-eps*) specifically for engineering applications to lost-foam “eps” pattern mold design, and optimization of both the pattern blowing and steam-fusing cycles. A successful mathematical tool will help foundry engineering staff form lost-foam patterns with more uniform properties (e.g., density and fusion), thereby reducing casting scrap, energy consumption, and lowering environmental releases as a result of significantly fewer defective castings. Additionally, future castings can be produced that are capable of satisfying new demands on ‘power density’ to meet stringent fuel mileage and emission requirements.

Executive Summary: This Final Technical Report presents results obtained during FY 2001/2002 from a DOE-sponsored, foundry industry Project to enable engineering of lost foam patterns using advanced computer modeling (CFD). During FY 2001 this experimental and analytical Project developed and validated a new CFD software package, *Arena-flow-eps* for modeling the blowing of lost foam patterns. New fundamental experimental data were obtained, such as pre-puff size distributions. Experiments were conducted in prototypical lost foam tooling to quantify the three-dimensional filling of beads from individual guns into complex-geometry tooling. The *Arena-flow-eps* software was found to be in excellent agreement with this new data. The software was subsequently applied to a complex production lost foam pattern, a GM cylinderhead section. The software simulated blowing the pattern with no numerical difficulty in about 1-day on a Pentium-4 class computer workstation, and reveals a complex bead-filling pattern. *Arena-flow-eps* can determine where individual fill guns deliver their beads. Engineers can now use this new “math-based” modeling to ensure cost- and energy-effective tooling designs: the optimum location and number of fill guns, gun pressure/cycle parameters, and tool vent sizing and distributions.

During FY2002 *Arena-flow-eps* modeling capability was extended greatly, to also compute the pattern-forming thermal cycle. An energy conservation equation was added for the steam including wall (tooling) heat transfer and bead thermal capacity. During steam fusion, the CFD computations reveals three-dimensional, transient, steam flow into the packed bead ‘bed’ within the tooling, the swelling of beads with a corresponding loss of porosity for steam flow as each local region reaches the ‘glass transition temperature’, bead and steam temperatures throughout the mold, and a localize ‘fusion’ index at the end of cycle.

Fundamental validation and verification (V&V) studies have been performed using known analytical solutions, and grid convergence studies. The Graphical User Interface (GUI) now includes all thermal input parameters, such as steam and bead specific heats, bead swell-rate parameters. Graphical output was added for the new thermal computational variables, e.g. bead temperatures.

In summary, this focused two-year CFD Project has led to a new commercial software package (*Arena-flow-eps*) for advanced engineering of lost foam pattern formation. Specifically, the new software models all fluid/particle/thermal phenomena during both the bead-blowing and the pattern-fusing cycles – within a single, integrated computational tool. Engineering analysis with *Arena-flow-eps* will enable foundries to now obtain desirable foam pattern characteristics in a reliable (consistent) manner, aided by an understanding of the fundamental fluid/thermal physics of the process. This will lead to significant reductions in casting scrap and energy usage, as well as enable future castings to satisfy stringent requirements on high-power-density and low-emissions in tomorrow's automotive and watercraft engines. During FY 2003 plans are to work with the University of Alabama Birmingham (UAB) and industry (GM, Foseco) to further improve modeling (e.g., bead compaction, swelling and fusion), as well as to further validate the software with advanced measurement instrumentation of thermal and fusion characteristics. Commercial usage of the *Arena-flow-eps* software is now occurring within the industry; this includes General Motors and Foseco-Morval, who are leading the field for designing and producing tomorrow's lost foam castings for diverse automotive and watercraft applications.

Background: In expandable polystyrene (eps) molding, or lost foam casting, a thermoplastic material, in bead form, is blown into a mold, and then fused by steam-injection to form a lightweight replica of the casting. This project has successfully completed development of an innovative, gas-solid (two-phase) computational fluid dynamics (CFD) computer program for modeling and simulation of both pattern-forming cycles: the bead blowing and the steaming or 'fusion.'

During FY2001 numerical modeling was directed towards the bead blowing, or filling phase. During FY2002 modeling was extended to include the steaming phase during which beads are thermally-expanded and "fused." The CFD approach uses a revolutionary multiphase-particle-in-cell (MP-PIC) numerical methodology. Its Eulerian-Lagrangian approach models the air or steam as a continuum fluid, and the eps beads as discrete particles with a user-specified size (and density) distribution. This provides the ability to calculate subgrid characteristics of the beads such as local wall reflections and distinct interfaces, e.g., unfilled, or poorly filled regions of the mold during filling. During steam fusion, the CFD computation reveals the three-dimensional, transient, steam flow into the packed bead 'bed', the swelling of beads with a corresponding loss of porosity for steam flow, bead and steam temperatures throughout the mold, and a localized 'fusion' index at the end of the cycle.

1.0 Overview of Project Accomplishments During FY2001

New fundamental data were generated for basic properties of pre-puff material, fill guns and lost-foam tooling. Data were taken to quantify pre-puff size distribution, fill gun performance characterization, and the air-flow-resistance of tooling vents. Several different experiments have been conducted in production lost-foam tooling to quantify the bead filling patterns

within complex geometries. Experiments include thin-to-thick (4-24 mm) plates and the “GM box” patterns (also used for x-ray imaging in associated DOE projects).

The *Arena-flow-eps* software is now a complete commercial package for simulating lost foam pattern blowing and steaming. The software has proven robust and easy to use with a complete graphical user interface (GUI). The *Arena-flow-eps* software package consists of: (1) an automatic mesh generator using import of 3D solid models of the tooling, (2) a “flow solver” for transient, three-dimensional air flow with discrete pre-puff particles (from ~150,000 to > 1,000,000), and (3) a powerful graphics visualization capability (GMV) developed especially for particle flows. Code assessments calculations were made against the industry-consortium sponsored experiments; and excellent agreement was obtained for pre-puff filling behavior. These calculations used the basic pre-puff data and fill gun boundary condition information obtained under this DOE-sponsored Project. Finally, the *Arena-flow-eps* software package was applied to a General Motors’ production cylinderhead foam pattern with 13 fill guns. A technical task was completed to extend *Arena-flow-eps*’s models towards simulating the pattern steaming (fusing) process during FY2002

2.0 Overview of Project Accomplishments During FY2002

Modeling and assessment enhancements made to *Arena-flow-eps* during FY 2002 have enabled simulation of the second-phase of lost foam pattern forming – the bead ‘fusion cycle’ required to have a structurally formed pattern. During the ‘fusion cycle’ steam is forced into the tooling through the vents; steam flow can be cross-steamed from one side to an other, or ‘autoclaved’ with steam forced into both sides of the tooling. Venting thus plays a dual role in the pattern forming process; first it allows air egress during bead (prepuff) filling (blowing), and then, it allows steam ingress during fusion. The *Arena-flow-eps* software can now be used to optimize venting sizes and locations considering the needs of both the blowing and steaming cycles.

As steam moves into the tooling cavity and through the packed-bed of beads, their temperature rises; at the glass-transition temperature (~ 120 C) rapid swelling occurs. The swelling causes a localized reduction and/or blockage of the steam flowrate. In a 3D production pattern the steam’s motion can become quite complex. Continued energy input via steam flow, molecular diffusion (conduction) and wall heat transfer causes a further rise in bead temperatures and ultimately local ‘fusion’ of the beads. The local distribution of bead temperatures and time-above-glass-transition-temperature throughout the entire mold can become quite three-dimensional. This means the local extent of bead fusion may be correspondingly complex (or incomplete). Measurement techniques to determine the extent of local fusion in patterns is currently under investigation by a parallel DOE-sponsored Lost Foam Consortium. Real-time x-rays during metal fill (pattern evaporation) conducted by UAB and GM have conclusively shown the importance to metal motion and defect formation of a pattern’s local fusion and surface permeability. Thus, engineering studies with *Arena-flow-eps* can help ensure foam patterns are formed with more precise and desirable (uniform) properties for both density and fusion. During FY 2003 plans are in place to work with UAB and industry (GM, Foseco) to further improve modeling (e.g., bead compaction, swelling and fusion), as well as to validate the software’s thermal models with new instrumentation.

Before any model development was undertaken, *Arena-flow-eps* development staff formally solicited input from researchers and industry experts to identify the important phenomena required to be included. The principal phenomena of importance during the fusion cycle are the following:

1. local 3D steam temperatures
2. local 3D steam flow rates
3. steaming BCs in both cross-mode and autoclave
4. bead thermal behavior
5. bead swell rates
6. bead glass transition temperature
7. local fusion or porosity 'index'

The above phenomena modeling necessitated the addition to *Arena-flow-eps* of both steam and particle (prepuff) energy conservation equations, including wall heat transfer boundary conditions. The equations set being solved, and fundamental validation studies are provided in a separate technical report ("Expanded Polystyrene Fusion", D. Snider, *Arena-flow*, LLC Technical Note 53). That report presents the partial differential equations solved for the fluid (steam) continuum, for each particle, for the tool wall heat transfer, for bead swelling, and for the local permeability reduction. It also presents results from two 'fusion-thermal-wave' validation calculations, as well as numerical sensitivity studies on time-step-size and meshing.

3.0 SUMMARY: Integrated Capabilities of the new *Arena-flow-eps* Engineering Software Package

This Topical Report presents results obtained during FY 2001/2002 from a DOE-sponsored, foundry industry Project to enable engineering of lost foam patterns using advanced computer modeling (CFD). During FY 2001 this experimental and analytical Project developed and validated a new CFD software package, *Arena-flow-eps* for modeling the blowing of lost foam patterns. New fundamental experimental data were obtained, such as pre-puff size distributions. Experiments were conducted in prototypical lost foam tooling to quantify the three-dimensional filling of beads from individual guns into complex-geometry tooling. The *Arena-flow-eps* software was found to be in excellent agreement with this new data. The software was subsequently applied to a complex production lost foam pattern, a GM cylinderhead section. The software simulated blowing the pattern with no numerical difficulty in about 1-day on a Pentium-4 class computer workstation, and reveals a complex bead-filling pattern. *Arena-flow-eps* can determine where individual fill guns deliver their beads. Engineers can now use this new "math-based" modeling to ensure cost- and energy-effective tooling designs: the optimum location and number of fill guns, gun pressure/cycle parameters, and tool vent sizing and distributions. Finally, a "tutorial" paper was written on how to use the *Arena-flow-eps* software for engineering design and trouble-shooting on production lost foam patterns.

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flow as each local region reaches the ‘glass transition temperature’, bead and steam temperatures throughout the mold, and a localized ‘fusion’ index at the end of cycle. Fundamental validation and verification (V&V) studies have been performed using known analytical solutions, and grid convergence studies. The Graphical User Interface (GUI) now includes all thermal input parameters, such as steam and bead specific heats, bead swell-rate parameters. Graphical output was added for the new thermal computational variables, e.g. bead temperatures.

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Expanded Polystyrene Fusion

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Introduction

This paper presents *Arena-flow* predictions of the fusion phase of lost-foam pattern production. *Arena-flow* is a particle-fluid math based tool for predicting the blowing and fusion process in foam pattern making. The premise behind math based tools is that if fundamental physics are understood and modeled well, then the math will take care of the details in calculating a wide variety of complex problems.

There is a general understanding of pre-expanded polystyrene (eps) expansion during fusion process; however, the fundamental physical behavior of gas flow, heat transfer, and of eps expansion from heating is not well known. *Arena-flow* makes use of currently available physical models for calculating the fusion process. The calculation presented here is for a simple test section. The calculation mold is described as an experiment. As far as *Arena-flow* is concerned, a simple geometry is no more difficult to solve than a complex geometry. However, because of the sparse fundamental physical data on fusion (thermal/hydraulic/mechanical) the simple pattern is an excellent experiment which can provide a wealth of data for verifying the current *Arena-flow* models, and data to advance the understanding of physics leading to more accurate math models.

One of the best uses of *Arena-flow* calculations is to provide provide insight into the fusion process. This is true for the calculations presented in this paper. The accuracy of the fusion calculations cannot be quantified without comparing with experimental data. The proposed simple pattern provides an easy to measure verification. If experimental data are acquired which modify an existing physical model or lead to new physical models, the accuracy of the calculations will improve.

In this study the term "fusion" is used loosely. In the foam casting industry, it has different meanings to different people. The basic term "fusion" refers to the expansion of eps and the adhesion of beads forming a structurally solid pattern. In this study, "fusion" is used to express the expansion of heated eps and the implicit cohesion of the beads.

This study considers four variational calculations. The study examines the influence of the feed temperature and the maximum expansion of eps during heating. The two feed temperatures are 390 K and 533 K. The maximum eps expansion (parameter in the eps bead expansion model) is 93% and 97%. There are many independent physical variables controlling foam fusion, and the influence of each parameter is relegated to future study.

Lost foam pattern geometry

The simple rectangular brick mold shown in Fig. 1 is used. If the shown geometry is an experiment, the pattern will be instrumented to measure pressure drops, temperatures and gas flow rate.

The mold shown in Fig. 1 is 2.5 cm x 2.5 cm wide and 5 cm high. The bottom of the mold has a screen cover giving a 10% open area. A uniform mesh screen is used to give a uniform inlet flow. This makes a simpler boundary condition than discrete vents which produce jets and give more complex data to analyze. The walls will be made of glass or a high-temperature resistant plastic. The transparent walls allow high-speed videos of the eps behavior and also

gives thermally insulated walls. Thermally insulated walls isolates the energy transport to the energy flowing through the vent.

Figure 1. Test mold.
Figure 1. The geometry of the foam pattern.

Fluid energy equation

The fluid internal energy equation is

$$\frac{\partial}{\partial t}(\theta_f \rho_f e_f) + \nabla \cdot (\theta_f \rho_f e_f \mathbf{u}_f) + p \nabla \cdot (\theta_f \mathbf{u}_f) + p \frac{\partial \theta_f}{\partial t} = \Phi + Q_w + Q_c + Q_j - Q_p + \Gamma_f h_{fp} \quad (1)$$

where θ_f is the fluid volume fraction, ρ_f is the fluid density, e_f is the fluid internal energy, $\mathbf{u}_f$ is the fluid velocity, p is the fluid pressure. Q_w is the heat flux from solid structures; Q_c is an internal heat source such as chemical reaction; Q_p is the heat flux from particles to fluid; and Q_j is molecular and turbulent diffusion of heat. The viscous dissipation is Φ . The rate of fluid mass phase change per volume is Γ_f . The heat diffusion is

$$Q_j = \nabla \cdot (k_f \theta_f \nabla T_f) \quad (2)$$

Heat transfer from solid structures is

$$Q_w = \int_{A_w} h_q (T_w - T_f) dA_w \quad (3)$$

which is discretely modeled as

$$Q_{w\xi} = \frac{1}{\Omega_\xi} \sum_{w\xi} h_q (T_w - T_f^{n+1}) A_{w\xi} \quad (4)$$

The particle internal energy transfer is

$$Q_{p\xi} = \frac{1}{\Omega_\xi} \sum S_{\kappa\xi} m_{p\kappa} [\dot{e} - D_{p\kappa} (u_{f\kappa} - u_{p\kappa})^2] \quad (5)$$

where $S_{\kappa\xi}$ is the interpolation operator between particle κ and control volume cell ξ . The second expression in brackets is the energy from particle to fluid drag. The energy transfer is

$$\dot{e} = \frac{1}{m_p} \delta m_p h_{fp} - \frac{A_p}{m_p} h_{qp} (T_f - T_p) \quad (6)$$

The A_p is the particle surface area, m_p is the particle mass, h_{qp} heat transfer coefficient, T_f is the fluid temperature at the particle location, and T_p is the particle temperature. The δm_p is the particle phase change from solid to fluid and h_{fp} is the latent heat.

Particle energy equation

A particle is approximated as having a uniform temperature which gives a lumped-heat-capacitance energy equation. The particle energy equation is

$$\dot{e} = \frac{A_p}{m_p} h (T_f - T_p) - \frac{1}{m_p} \delta m_p h_{fp} \quad (7)$$

where A_p is the particle surface area, h is the heat transfer coefficient, and T_f and T_p are the fluid and particle temperatures, respectively. The last term in Eq. (7) is the energy from phase change from solid to fluid. The δm_p is the loss of mass from the particle and h_{fp} is the latent heat. If the particle grows from "condensation" onto the particle, the condensing fluid mass, δm_p , must loose energy to the particle (the last term in Eq. (7) will be positive). If the particle is vaporizing, the particle must supply energy to vaporize δm_p (the last term in Eq. (7) will be negative). The equations presented so far do not consider a chemical reacting particle.

If the particle is spherical or is represented by an effective radius $\bar{r}$, the area is

$$A = \frac{3\phi\Omega_p}{\bar{r}} \quad (8)$$

where ϕ is the sphericity factor. For a sphere, $\phi = 1$.

The particle energy is

$$\dot{e} = C_p \frac{dT_p}{dt} \quad (9)$$

where C_p is the particle specific heat at constant volume. The particle energy equation, without mass transfer is

$$\rho_p C_p \Omega_p \frac{dT_p}{dt} = h A_p (T_f - T_p) \quad (10)$$

where ρ_p is the particle density, Ω_p is the particle volume, The implicit numerical approximation for the particle energy equation for the finite time step Δt is

$$T_p^{n+1} = \frac{T_p^n + \alpha_p T_f}{1 + \alpha_p} \quad (11)$$

where $\alpha_p = \frac{h A_p \Delta t}{\rho_p C_p \Omega_p}$, and $n+1$ is the new time and n is the old time.

The numerical approximation assumes that there is sufficient fluid to continuously supply heat at fluid temperature T_f . For a liquid with a large density and heat capacity or for few particles, this is a good assumption. However for a gas and/or dense particle flow, the assumption is poor. The solution from Eq. (11) can extract more energy from the fluid than exists in the fluid. One method of handling dense particles or low gas heat capacity, is to have a small calculation time step. Another approach, used in *Arena-flow*, is to implicitly include the gas in the particle energy equation. The volume of gas associated with each particle is

$$\Omega_{fp} = \frac{\theta_{f\xi} \Omega_\xi}{N_{p\xi}} \quad (12)$$

where $\theta_{f\xi}$ is the fluid volume fraction in cell ξ , Ω_ξ is the volume of cell ξ , and $N_{p\xi}$ is the number of particles in cell ξ .

Figure 2. Simple model for Lagrangian particles with with a Lagrangian fluid.

The particle energy equations are ordinary differential equations in a Lagrangian reference, and it is desirable to maintain the Lagrangian calculation. In doing so, it is assumed that the gas volume associated with each particle moves in a Lagrangian frame of reference with the particle. The Lagrangian fluid energy equation is

$$\rho_f C_f \Omega_{fp} \frac{dT_f}{dt} = -h A_p (T_f - T_p) \quad (13)$$

where ρ_f is the particle density, C_f is the particle specific heat at constant volume. The dominate energy transfer is heat from particle to gas. The implicit numerical approximation for the Lagrangian fluid energy equation for the finite time step Δt is

$$T_f^{n+1} = \frac{T_f^n + \alpha_f T_p^{n+1}}{1 + \alpha_f} \quad (14)$$

where $\alpha_f = \frac{h A_p \Delta t N_{p\xi}}{\rho_f \theta_{f\xi} \Omega_\xi C_f}$, and $n+1$ is the new time and n is the old time.

Inserting the fluid temperature from Eq. (14) into the particle energy equation, Eq. (10), the particle energy equation is

$$T_p^{n+1} = \frac{T_p^n + \frac{\alpha_p}{1 + \alpha_f} T_f^n}{1 + \frac{\alpha_p}{1 + \alpha_f}} \quad (15)$$

The number of particles in cell ξ , is

$$N_{p\xi} = \frac{\theta_{p\xi} \Omega_\xi}{\Omega_p} \quad (16)$$

where the particles are all the same volume. For a particle size distribution, the number of particles in a cell is an approximation. The fluid constant is

$$\alpha_f = \frac{h A_p \Delta t}{m_p C_f} \frac{\rho_p \theta_p}{\rho_f \theta_f} \quad (17)$$

For dilute particle flow or a fluid with a high heat capacitance, α_f is small and the particle energy equation Eq. (17) reduces to Eq. (11).

Coupling particles into the fluid energy equation

The Eulerian fluid equation is implicitly solved with the particles. Putting Eq.(11) into Eq. (5)

$$Q_{p\xi} = \frac{1}{\Omega_\xi} \sum S_{\kappa\xi} \left[\frac{A_p h_{qp} ((T_f^{n+1} - T_p^{n+1}) - \delta m_p h_{fp})}{1 + \alpha} - m_p D_{p\kappa} (u_{f\kappa} - u_{p\kappa})^2 \right] \quad (18)$$

The fluid temperature can be cast into an energy and implicitly solved with new-time energy terms.

$$Q_{p\xi} = \frac{1}{\Omega_\xi} \sum S_{\kappa\xi} \left[\frac{A_p h_{qp} \frac{e_f^{n+1}}{C_{Vf}}}{1 + \alpha} \right] - \frac{1}{\Omega_\xi} \sum S_{\kappa\xi} \left[\frac{A_p h_{qp} T_p^{n+1} - \delta m_p h_{fp}}{1 + \alpha} - m_p D_{p\kappa} (u_{f\kappa} - u_{p\kappa})^2 \right] \quad (19)$$

Arena-flow units

e	Internal energy	J/kg
$\dot{e}$	Rate of change of internal energy	J/kg-s
C_v	Specific heat at const volume	J/kg-K
T	Temperature	K
h_q	Heat transfer coefficient	J/s-m ² -K
k	Thermal conductivity	J/s-m-K
δm_p	Rate mass phase change	kg/s
Γ_f	Rate mass phase change per volume	kg/m ³ -s
h_{fp}	Enthalpy (latent heat)	J/kg
D	Drag coefficient	1/s

Particle-to-fluid heat transfer coefficient

The heat transfer between gas and particles is modeled by

$$Q = A_p h (T_p - T_f) \quad (20)$$

where A_p is the particle surface area, T_p is the particle temperature, and T_f is the fluid temperature at the particle location. The heat transfer coefficient is an empirical equation for all but very simple cases. Because the heat transfer coefficient is empirical, its accuracy is limited to the range of conditions for the experiments from which it was generated. Empirical equations have traditionally been in the form of a combination of Reynolds number, fluid properties (usually Prandtl number) and geometry parameters. *Arena-flow* uses a generic form of the heat transfer coefficient

$$Nu = C_0 Re^{n_1} Pr^{0.33} + C_1 \quad (21)$$

The Reynolds number is

$$Re = \frac{\rho_f |U_f - U_p| D_p}{\mu_f} \quad (22)$$

where ρ_f is the fluid density, μ_f is the fluid viscosity, D_p is the particle effective diameter, and U_f and U_p are the fluid and particle velocities, respectively.

The Nusselt number is

$$Nu = \frac{h D_p}{k_f} \quad (23)$$

where k_f is the fluid conductivity.

The constants in Eq. (21) are user-supplied values, with the *Arena-flow* default values based on McAdams (1954) and Kramers (1946), of

C_0	0.3
C_1	0.98
n_1	0.5

Eq. (21), in terms of the heat transfer coefficient, is

$$h = (C_0 Re^{n_1} + C_1) k_f / D_p \quad (24)$$

This study uses $C_0=0.3$, $C_1=0$, and $n_1=0.5$.

Polystyrene bead expansion

Pre-puff polystyrene (eps) expands when the bead temperature reaches or exceeds the glassification temperature, T_{glass} . If the particle temperature exceeds the eps glass temperature ($T_p > T_{glass}$) then the expansion rate of eps is approximated by

$$\frac{dr}{dt} = C(r_{max} - r) \quad (25)$$

The numerically approximated radius growth rate over time interval Δt is

$$r^{n+1} = \frac{r^n + C r_{max} \Delta t}{1 + C \Delta t} \quad (26)$$

where r is the eps radius and $n+1$ is the new time and n is the old time. The r_{max} is the maximum particle expansion which is specified by a factor, c_2 , multiplied by the mean particle radius, $\bar{r}$.

$$r_{max} = c_2 \bar{r} \quad (27)$$

The expansion constant is

$$C = c_1 \Delta T \Delta \theta \quad (28)$$

where

$$\Delta \theta = \theta_{max} - \theta, \quad (29)$$

$$\Delta T = T_p - T_{glass} \quad (30)$$

and θ is the particle volume fraction and θ_{max} is the maximum particle volume fraction.

In this study $T_{glass}=373$ K, $c_1=10 \text{ s}^{-1}$, $c_2=2.5$, and $\theta_{max}=0.93$ and 0.97 .

The surface area exposed to gas decreases as the eps beads plastically fuse together, as illustrated in Fig. 3. Initially beads contact at single points (or no contact) with its neighbors. The heat transfer surface area is the surface of a sphere. As beads expand, the flow channel decreases and the bead form together and the surface area in contact with gas decreases. The

surface area in particle-to-fluid heat transfer equations are multiplied by an area adjustment factor. The factor is

$$f = \begin{cases} 1 & \theta_p \leq \theta_{cp} \\ \theta_g / (1 - \theta_{cp}) & \theta_p > \theta_{cp} \end{cases} \quad (31)$$

Figure 3. Heat transfer area from gas to eps. Left: Eps beads before expansion.
Right: Eps beads expanding into neighbor beads.

Table 1. Calculation parameters

Arena version=3.00
Calculation time step (dynamically adjusts)=0.000200 s from 0. s to 3.000000 s
Equation of state = Incompressible
Number of x grid cells = 10
Number of y grid cells = 10
Number of z grid cells = 25
x range = 0.000154 to 0.024999 m
y range = 0.000000 to 0.025000 m
z range = 0.000000 to 0.049999 m
Time wt advection and diffusion = 1.000
Time wt on particle velocity in interface drag = 1.000
x gravity = 0.000000 m/s ²
y gravity = 0.000000 m/s ²
z gravity = -9.800000 m/s ²
Fluid viscosity = 0.000019 kg/m s
Isothermal flow = No
Fluid thermal conductivity = 0.310000 J/m s
Fluid Specific heat at constant volume = 1006.000000 kg/m s
Fluid density = 0.900000 kg/m ³
Close pack volume fraction = 0.5500
Multiply drag coefficient = 1.000
Normal wall restitution = 0.20
Tangential wall restitution = 0.70
Particle to particle restitution = 0.00
Drag model = Ergun
Use particle-to-particle drag = No
Feed Gaussian distribution = Yes
Gaussian bounce at wall = Yes
Inviscid flow = No
Inviscid wall boundaries (slip) = No
Maximum pressure residual = 1.00e-08
Maximum velocity residual = 1.00e-08
Maximum volume residual = 1.00e-08
Turbulence model = None
Blend 1st and 2nd order advection = 100% 1st order 0% 2nd order
Particle normal stress model constants
Constant multiplier (Ps) = 10.00 Pa
Power on volume fraction (b) = 3
Denominator limiter eps (e) = 1.000e-07
Particle species = 1
Effective particle radius = 200.000000 to 400.000000 µm
Particle density = 48.000000 to 48.000000 kg/m ³
Sphericity = 1.0000006.2
Thermal conductivity = 0.500000 J/m s
Specific heat = 1500.000000 kg/m s
Glass temperature = 373.000000 K
Max radius (x ave radius) = 2.500000
Max volume fraction = 0.9300
Expansion rate coef = 10.000000 1/s
Fluid to wall heat transfer coefficient
c0 = 0.023000
c1 = 0.000000
n1 = 0.800000
n2 = 0.330000
Fluid to particle heat transfer coefficient
c0 = 0.300000
c1 = 0.000000
n1 = 0.500000

Arena-flow calculation

The flow, and energy transfer in a rectangular brick with and without expanded polystyrene is calculated. The initial gas and eps bead temperature in the mold is 310 K. The gas, in the calculation is hot air. This is a significant difference from the industrial steaming of eps foam. One advantage of using saturated steam is that the steam maintains its temperature as it transfers heat to the eps (at constant pressure). Once latent heat of vaporization is exhausted, the steam changes to single phase water. Further it is reported that steam permeates into the eps bead which enhances expansion. For model development and initial experiments, it is recommended to initially use heated air. The boundary conditions are constant gas pressure of 200 kPa at the bottom inlet, and constant pressure of 0 kPa at the top. Inlet gas temperatures of 390 K and 533 K were used. Calculation parameters are given in Table 1.

Note that graphs show the boundary conditions (outside the calculation domain). At the exit boundary, the temperature is 390 K, and it is shown on graphs. Because the flow is one-way through and out the mold, the exit boundary temperature does not influence the temperature in the mold.

Calculations are made with two bead expansion limits and two feed temperatures. One calculation uses $\theta_{max}=0.93$ and other uses $\theta_{max}=0.97$. The two limits are not hard numbers. That is, the numerical solution allows beads to expand *approximately* to the set maximum volume fraction. Both limits give a small minimum gas flow areas which are 3% and 7%.

Energy transport in an empty mold

The transient temperature at vertical locations in an empty mold are shown in Fig. 4. The hot gas rapidly heats the gas in the 5 cm thick mold, and the mold temperature reaches the gas feed temperature in 3 ms.

Figure 4. Transient temperature in empty mold. No wall heat transfer.

Energy transport

Maximum eps volume fraction of 97% and 533 K gas temperature

Figure 5 shows the particle field during hot air fusion. The maximum eps expansion volume fraction is 97%. The inlet gas temperature is 533 K. The eps particle field shows that the bottom eps quickly expands and closes off flow of hot gas. The rapid bead expansion is further seen in Fig. 6 which shows the transient eps volume fraction at the bottom of the mold and at 2 cm from the bottom. The depth of eps fusion (expansion) is very shallow as seen in Fig. 7.

Fig. 8 shows the transient gas and eps temperatures. The temperatures of two discrete eps beads are shown. Near the hot gas inlet, the gas temperature quickly rises and is followed by the eps temperature as heat is transferred to the eps. When the eps temperature exceeds the glass temperature, the beads swell and block the gas flow. With blocked gas flow, the gas temperature loses heat to the beads and the gas temperature curve turns over and decreases. Energy continues to be transferred between eps and gas until a common temperature is reached.

Fig 9 shows that the gas temperature increases all along the mold, from the initial influx of hot gas. The particles follow the modest temperature rise and quickly reach the gas temperature. The decreases in gas velocity and the large pressure drop at the bottom of the mold are shown in Figs. 10 and 11, respectively.

Figure 5. Eps beads during fusion with hot air. Beads are colored by local eps volume fraction. Calculation with $\theta_{max}=0.97$, and 533 K gas temperature.

Figure 6. Eps volume fraction. Maximum eps expansion is 97%, and 533 K gas temperature.

Figure 7. Eps volume fraction distribution at vertical locations in the mold. Maximum eps expansion is 97%, and 533 K gas temperature.

Figure 8. Gas and eps temperatures. Maximum eps expansion is 97%, and 533 K gas temperature.

Figure 9. Temperature distribution at vertical locations in the mold. Maximum eps expansion is 97%, and 533 K gas temperature.

Figure 10 Gas vertical velocity at locations in the mold.
Maximum eps expansion is 97%, and 533 K gas temperature.

Figure 11. Pressure at locations in the mold.
Maximum eps expansion is 97%, and 533 K gas temperature.

Maximum eps volume fraction of 93% and 533 K gas temperature

Figure 12 shows the eps volume fraction with a maximum eps expansion volume fraction of 93% and 97% with a gas feed temperature of 533 K. The maximum eps expansion is a parameter in the bead expansion model. The lower expansion limit, which gives less gas blockage, gives slightly deeper fusion (particle swell).

Figure 12. The eps volume fraction at 1s for a maximum eps expansion of 93% and 97% and 533 K gas temperature.

Maximum eps volume fraction of 93% and 390 K gas temperature

Figure 13 shows the eps expansion front at several times assuming a maximum eps expansion volume fraction of 93% and an inlet gas temperature of 390 K. The color, in Fig. 13, is local eps volume fraction with red being 100% and blue 50% volume fraction. The figure shows the progression of the fusion front moving up the mold. One obvious observation, compared to the previous calculation, is that using a lower gas feed temperature, the fusion extends deeper into the mold. Because of the complex interplay of physical behavior, it is not prudent to say that lowering the gas temperature generally gives deeper fusion. However, it is reasonable to say that because of the complex nature of the fusion process, the fusion in a new geometry or production part would be near impossible to predict without experiments or a math based tool.

Figure 14 shows the gas temperature. The eps temperatures are not shown, but the eps temperature follows the gas temperature with a slight lag. At the lower gas feed temperature, the beads do not swell as fast and gas penetrates deep into the pattern. The rate of increase in temperatures within the pattern slows with time as beads swell and block upstream gas flow. At 2 cm from the inlet, the eps reaches the glass temperature at 2.4 s, and at 3.2 cm eps, beads reach the glass temperature at 4.6 s. Fig. 15 shows the transient eps bead size for 5 discrete beads in the mold. The location of the eps beads is given in Table 2. When a bead reaches the glass temperature, it is calculated to rapidly expand. Because the rate-of-expansion-model is

partially driven by the temperature difference between eps and gas temperature, beads near the gas inlet have a faster rate of expansion than those deeper in the mold. The discrete beads chosen to be displayed were randomly selected. The eps bead at vertical height of 1 cm has considerably less expansion than the other beads shown. This occurs because beads around it have expanded to fill the space, and the regions has reached the 93% volume fraction limit. The gas and eps near the inlet, approach the inlet gas temperature and remain nearly constant.

Table 2. Location of eps beads shown in graphs.

x (cm)	y (cm)	z (cm)
0.9807	0.9626	0.0699
0.9436	1.0347	0.9809
1.0432	0.9544	2.0507
1.0354	1.0395	2.9676
0.9665	0.9633	4.0185
0.9621	1.0261	4.9493

Figure 13. The eps distribution. Color is local eps volume fraction. Maximum eps expansion is 93%, and 390 K gas temperature.

Figure 14. The gas and eps temperature. Maximum eps expansion is 93%, and 390 K gas temperature.

Figure 15. The transient bead expansion for discrete eps beads. Maximum eps expansion is 93%, and 390 K gas temperature.

Gas to eps drag model during fusion

Two fluid-to-particle drag models are used in *Arena-flow*. One is a Stokes-flow model. The other is a porous media model. The Stokes-based model is primarily applicable for distinct particles flowing in a fluid. The model is multiplied by a hindrance function which corrects Stokes-flow for high Reynolds number and concentration of particles. The Erguns equation porous media model was developed for porous media where the particles are not moving and where particles are densely packed.

For the fusion of eps, Erguns model is the better choice. Erguns model considers granular material with a characteristic diameter. The form of Erguns equation based on a granular material effective diameter breaks down for expanding eps. Fig. 16 shows packed eps at the start of fusion and at the end of fusion. At the start of fusion, eps beads are distinct spheres, and Erguns drag model is applicable. However as fusion progresses, the distinct beads disappear, and the flow path becomes narrow channels between fused polystyrene. The concept of an effective-diameter is taxed and Erguns equation is in question.

The flow paths between the expanding beads are complex winding channels. As the eps expands, flow area decreases which tends to increase the gas velocity. On the other hand the reduced area and increased flow drag reduces the gas mass flow rate.

Figure 16. Left: polystyrene at the start of fusion.
Right: polystyrene at end of fusion

At this time, it is not known how accurate Erguns drag equation or other models in the literature are for predicting drag between gas and expanding eps. The evaluation of accuracy of the drag models and their possible improvements requires experimental data. *Arena-flow* calculations using the current drag model and the bead-expansion-modeled, which closes the gas flow path, is expected to give a reasonable prediction of the gas flow rate.

Eps heat transfer

The particle energy equation in *Arena-flow* is a lumped-heat capacitance model. The lumped-heat capacitance model assumes that the particle is at a uniform temperature. This is true if the the energy transfer at the particle surface is much less than the heat transfer within the particle. If $hA \ll kr$, where hA is the surface heat transfer coefficient times surface area and kr is thermal conductivity times the particle length scale, then a lumped-heat capacitance model is a good approximation. The eps surface area is of order $\sim r^2$, and the requirement is $hr \ll k$. For small particles, the lumped-heat capacitance model is generally accurate.

For eps beads, which range in diameter from about 400 μm to 1100 μm , and which have a thermal conductivity on the order air, the approximation is taxed at high gas flow rates. As a

simple example, consider a 500 μm (diameter) eps bead in a 10 m/s air flow. The Reynolds number based on particle diameter is

$$Re = \frac{\rho_f |U_f| D_p}{\mu_f}$$

which is $Re=263$, for $\rho_f=1 \text{ kg/m}^3$, and $\mu_f=1.9 \times 10^{-5}$. The convective heat transfer model is

$$Nu = 0.3 Re^{0.5}$$

which gives $Nu = 4.86$. The Nusselt number definition is

$$Nu = \frac{h D_p}{k_f}$$

The fluid thermal conductivity is $k_f=0.3 \text{ J/s-m-K}$, and the heat transfer coefficient is $h=2920 \text{ J/s-m}^2\text{-K}$. The thermal conductivity of eps is on the order of air, $k_p=0.3 \text{ J/s-m-K}$. The surface heat flux measure is $hr = 1.46 \text{ J/s-m-K}$. Because the surface heat transfer parameter, hr is not smaller than the eps thermal conduction, the lumped-heat capacitance model is not a good assumption. As the beads swell, the approximation becomes worse.

The *Arena-flow* currently does not model the penetration of steam into eps beads. The transport of steam into the eps will tend to produce a uniform bead temperature. However there is no physical bases to expect the complex heating mechanism of steam transport across eps cell walls to be approximated well by the lumped-heat capacitance model.

Blockage of gas flow as beads expand

The *Arena-flow* bead expansion model allows the beads to expand to a maximum specified volume fraction. If the maximum eps volume fraction is 96%, then there is a 4% area for gas flow. The maximum expansion value is unknown and requires experimental evaluation. However, one can hold a polystyrene coffee cup tightly to their face and blow very hard into the cup . Very little air escapes through the foam walls. The calculation shows that with a maximum volume fraction greater than 93%, the eps expansion near the gas inlet quickly swells and can starves hot gas from reaching particles deeper in the mold. Fig. 17 (Benson, et. al. 2002) is a photograph of expanded beads at the pattern wall. From blockage seen in the photograph, it can be expected that beads away from the pattern surface are exposed to diminishing amounts of hot gas.

Figure 17. Fused eps beads. (Benson, et. al. 2002)

Numerical time step

It is a good practice to do a grid and time step study on numerical calculations. With the fast expansion of eps beads, the calculation time step is important. Fig. 18 shows calculations for 93% maximum eps expansion and a gas feed temperature of 390 K. The specified time step is the maximum time step during the calculation. *Arena-flow* may adjust the time step to a smaller value, during a calculation, based on velocities or other physical parameters.

Figure 18. Gas temperature calculated at 0.002 s and 005 s.

Fig. 16 shows calculations run at maximum time steps of 0.002 s and 0.005 s. The calculation at a larger time step predicts a slower rise in temperature within in the mold, compared to the small time step calculation. A variation between calculations is not unexpected because of the rapid expansion of a heated eps bead, and its coupled influence on other parameters. The calculated temperature difference is on the order of 5 K, which in itself is not significant. However, because the temperature curves flatten with time, a 5 K temperature variation near the glassification temperature makes significant difference on the rate of fusion. From a production point of view, if fusion is needed at 2 cm, then boundary conditions need to be modified to get a more reliable and repeatable fusion.

Concluding remarks

The gas flow, heat transfer and bead expansion is a complicated process and influenced by a host of physical parameters. For example, at a lower fluid feed temperature, beads expand slower and the gas penetrates deeper into the mold. However at a lower feed temperature, the fluid temperature decreases from heat transfer to eps as it moves through the mold, and the beads may not expand (eps below the glass temperature). This study took a rudimentary look at the heating and expansion of beads, and varied only a few parameters governing the process. The *Arena-flow* calculations provides insight into the fusion (eps expansion) process with the competing, interplay of parameters.

The *Arena-flow* calculations were for a simple geometry which could be used as an experiment mold. The simple geometry is easy to construct and instrument and allows for

direct visual observations, as well as traditional physical measurements. While the geometry is simple the physics is as complex as a commercial, production mold. However, in a production mold, with many vents and complex geometry, there will be added complexity from the interplay of complex gas flow paths with the fusion process.

The premise behind math based tools is that if fundamental physics are understood and modeled well, then the math description will take care of the details in calculating a wide variety of complex problems. The *Arena-flow* particle-fluid math based tool has been shown to predict well the blowing of eps beads, with excellent comparisons with experimental data. *Arena-flow* has much of the physics required to predict the flow/thermal/mechanical fusion process in pattern eps "fusion". Some of the *Arena-flow* models are incomplete, requiring experimental data to define the controlling variables and possibly identify new governing physics parameters. Integrated analysis and experiments, focusing on well defined fundamental physics, will provide improved or new math models which will increase computational accuracy.

References

McAdams, W. H., 1954, *Heat transmission*, 3d ed., McGraw-Hill Book Company, New York.

Kramers, H., 1946, "Heat transfer from spheres to flowing media," *Physica*, vol. 12, p.61.

Benson, R., Penumadu, D. and Michaels, R., 2002, "Quantification and standardization of pattern properties for the control of the lost foam casting process," Lost Foam Consortium Meeting, October, 22, 2002.