Uncertainty Quantification in Modeling of Solidification Processes

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Work sponsored by Bisland Doctoral Fellowship Program at Purdue University and Fiat-Chrysler Automotive

Leslie Comrie Seminar Series

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5 October 2016

Greenwich, UK

Predicting phenomena as single values

Observed phenomena do not have "single point values;" they cannot be predicted or measured with perfect certainty

Predicted performance levels cannot be absolutely assured, but only given in terms of probability

What is that level of uncertainty in the output?

Importance of that uncertainty depends on purpose of model

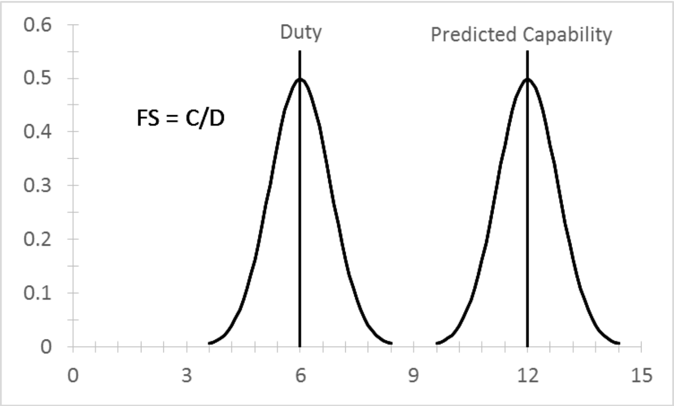
Three reasons for being concerned about uncertainty in our predictions

1. Limit to uncertainty of output

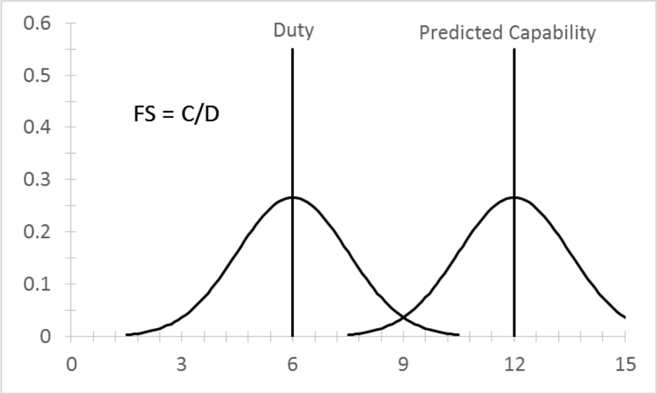
Question raised by Peter Quested (NPL, UK) at MCWASP (Aachen, 2000):

how much uncertainty in input data can we tolerate?

2. Design with factor of safety



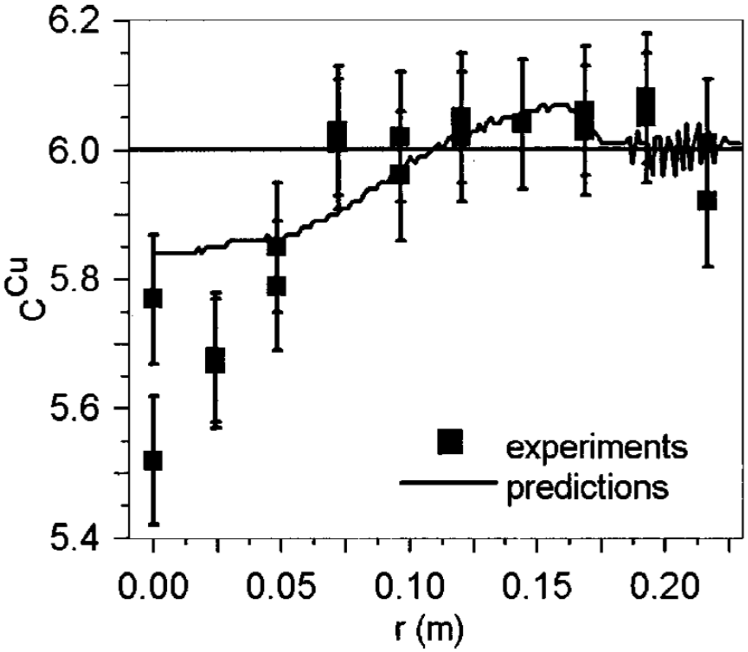
Expected duty of system = 6,
so design with a factor of safety of 2
(predicted capability = 12)



Proper value of factor of safety really informed by probability distribution functions of the predicted and the expected duty of system

Why are we concerned with uncertainty?

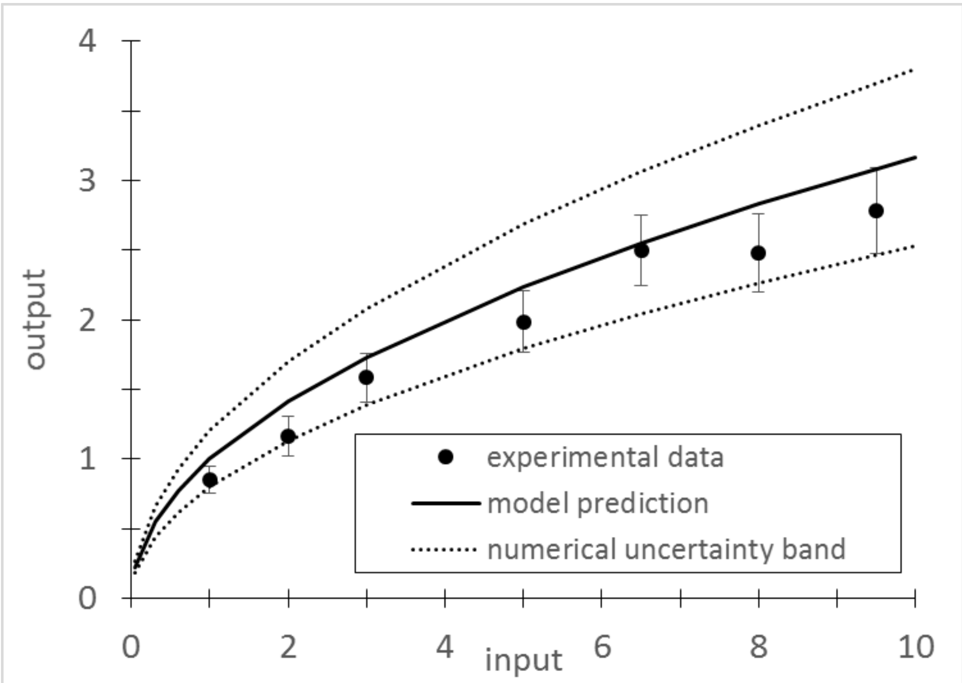
3. Validation of model predictions to experiments



Radial copper composition profile in DC cast ingot (Vreeman et al, *ASME JHT*, 2003)

What is the uncertainty in the model?

Do these data validate the model?



Agreement depends on uncertainties of experiment <u>and</u> model.

Sources of uncertainty: Numerical

Numerical uncertainty can usually be reduced by grid refinement, reduction of time step … within a given method

Exception: singularities

- discontinuous thermal boundary conditions
- leading edge of boundary layers
- crack tips (elastic stress model)

“Verification” uncertainty

Sources of uncertainty: Epistemic

Epistemic uncertainty = is the model physically correct?

Depends on:
state of knowledge of physical processes
what is included in our model

E.g., simple projectile motion – drag?
orbital mechanics – variable gravitational constants?

Best cure is better/more focused experiments to inform the model building

“Validation” uncertainty

Sources of uncertainty: Aleatoric

Aleatoric uncertainty =
- result of uncertainty of input values
- input is uncertain because it is variable or there is uncertainty in measurement

Material properties, initial and boundary conditions are model inputs with (hopefully) well-characterized probability distributions

What kinds of PDFs?

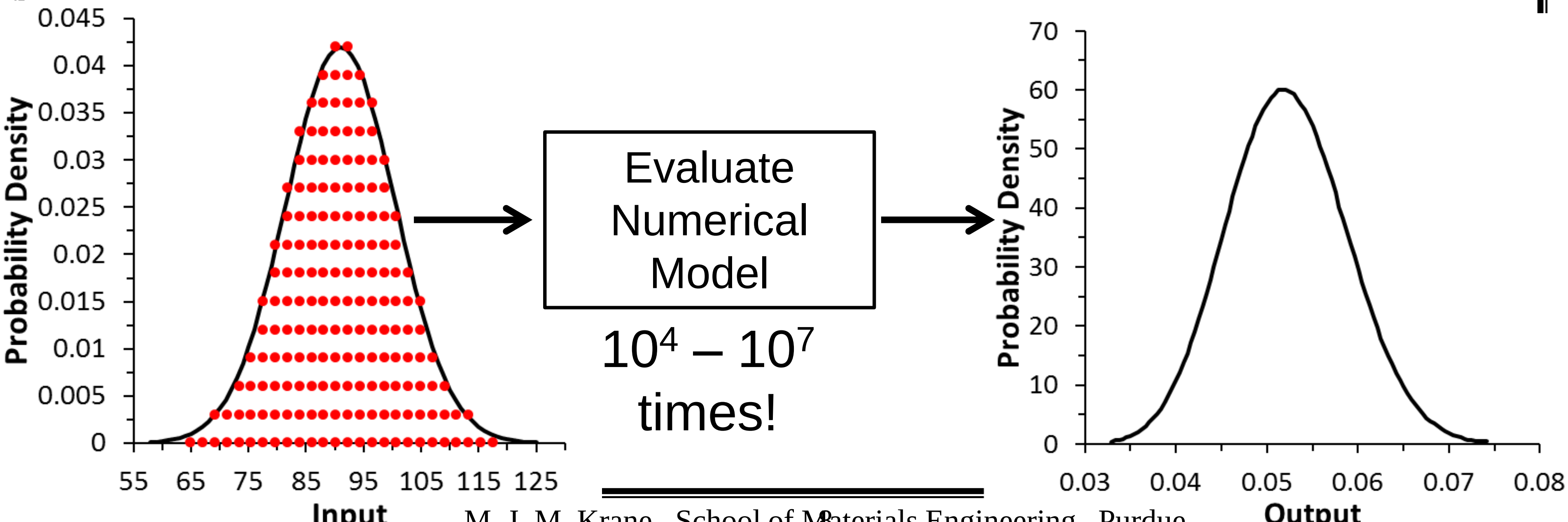
Gaussian, log-normal, uniform, scattered/discrete

what does your data look like?

We'll focus today on aleatoric uncertainty

Aleatoric Uncertainty Propagation by Brute Force: Monte Carlo Sampling

- Sampling methods produce probability density functions (PDFs) of outputs
- For each random value, evaluate model and calculate output parameter
- Method is simple and non-intrusive (model can be black box)
- Can become computationally expensive, is there a better way?



A less expensive approach: Use of a surrogate model

$q = f(p)$ p = input q = output $f(p)$ = model

random input (p) gives random output (q)

can build surrogate model (response surface), $\hat{f}(p)$,
that is <u>cheaper</u> than $f(p)$, from relatively few model evaluations

surrogate can be:
- subjected to Monte Carlo analysis;
- used to determine sensitivity of output to changes in input

usefulness of surrogate depends on how well $\hat{f}(p)$ mimics $f(p)$

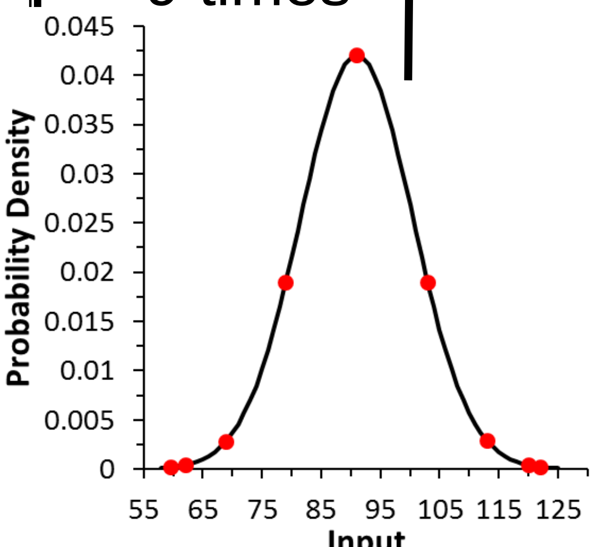
One example of “framework” software using surrogate model:
DAKOTA (Sandia National Labs)

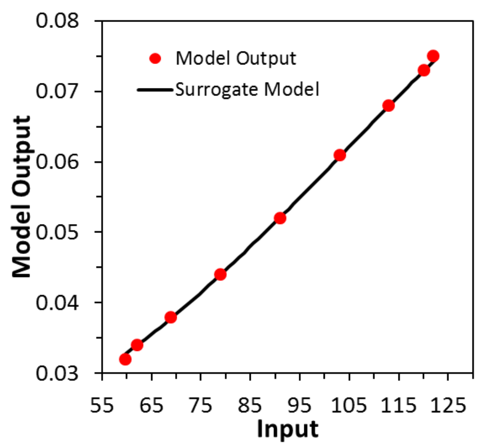
Building the Surrogate: Single Input

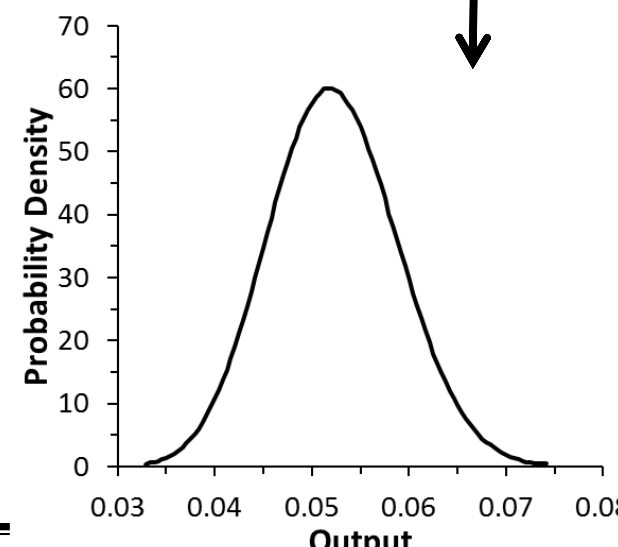
- Use of surrogate model is more computationally efficient
- Reduces the number of numerical model simulations by orders of magnitude

Evaluate Numerical Model → Generate Response Surface → Monte Carlo Sampling

9 times







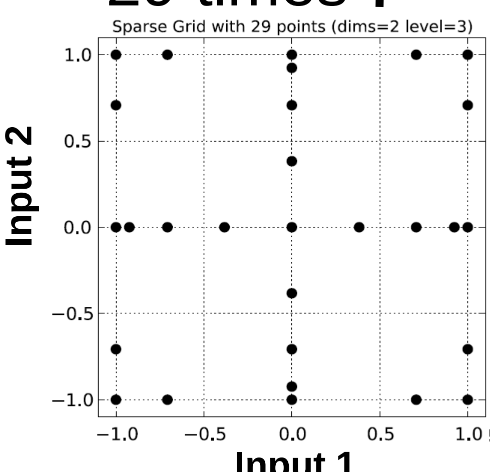
Building the Surrogate Model: Multiple Inputs

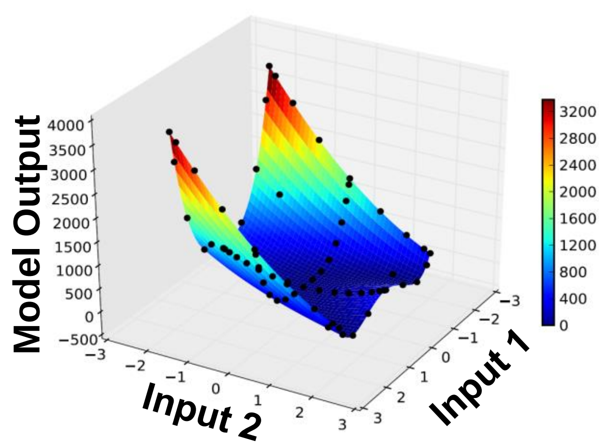
- More than one uncertain input can be propagated at a time
- Different polynomial orders can be used as a surrogate model
- Computational expense increases with polynomial order

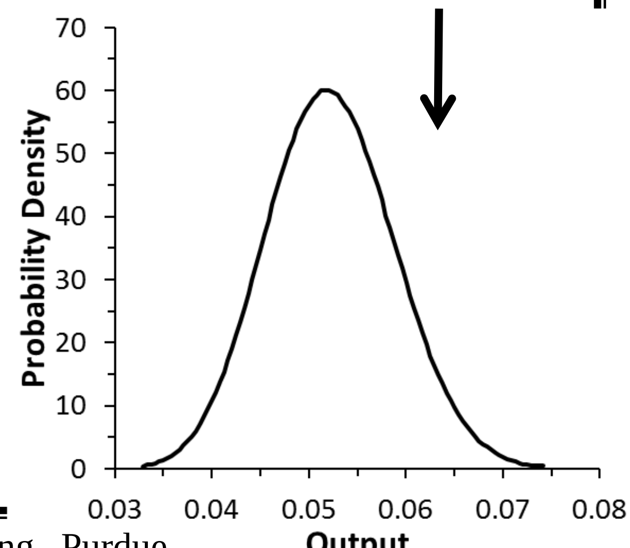
(Hunt et al., *Comp. Phys. Comm.*, 2015)

Evaluate Numerical Model → Generate Response Surface → Monte Carlo Sampling

29 times ↑







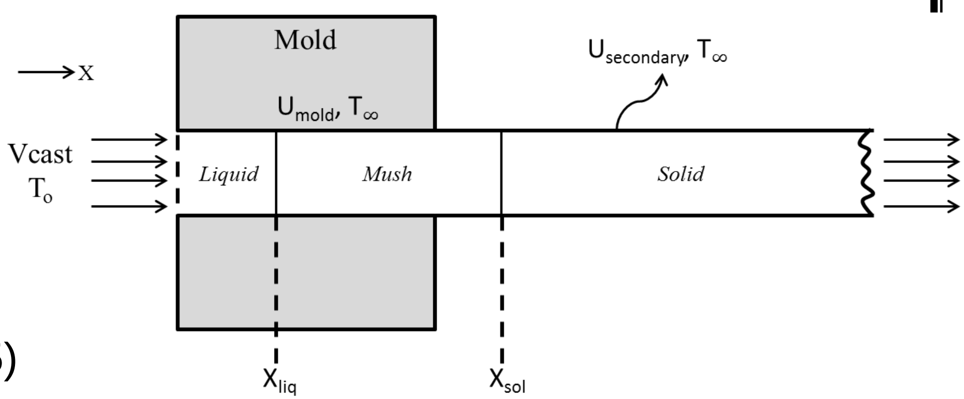
Uncertainty quantification with a surrogate

Another example of framework software:
PUQ (PRISM Uncertainty Quantification)
(Hunt et al., *Computer Physics Communications*, 2015)

- Freely available on Purdue's NanoHub (www.nanohub.org)
- Can download or run in cloud on NanoHub
- Non-intrusive:
  input = PDFs of input parameters
  output = surrogate model, PDFs of output parameters

- Example tools on NanoHub:
- Dislocation dynamics in nanocrystalline material
- 1D solidification model

(Fezi and Krance, MCWASP conf., 2015)



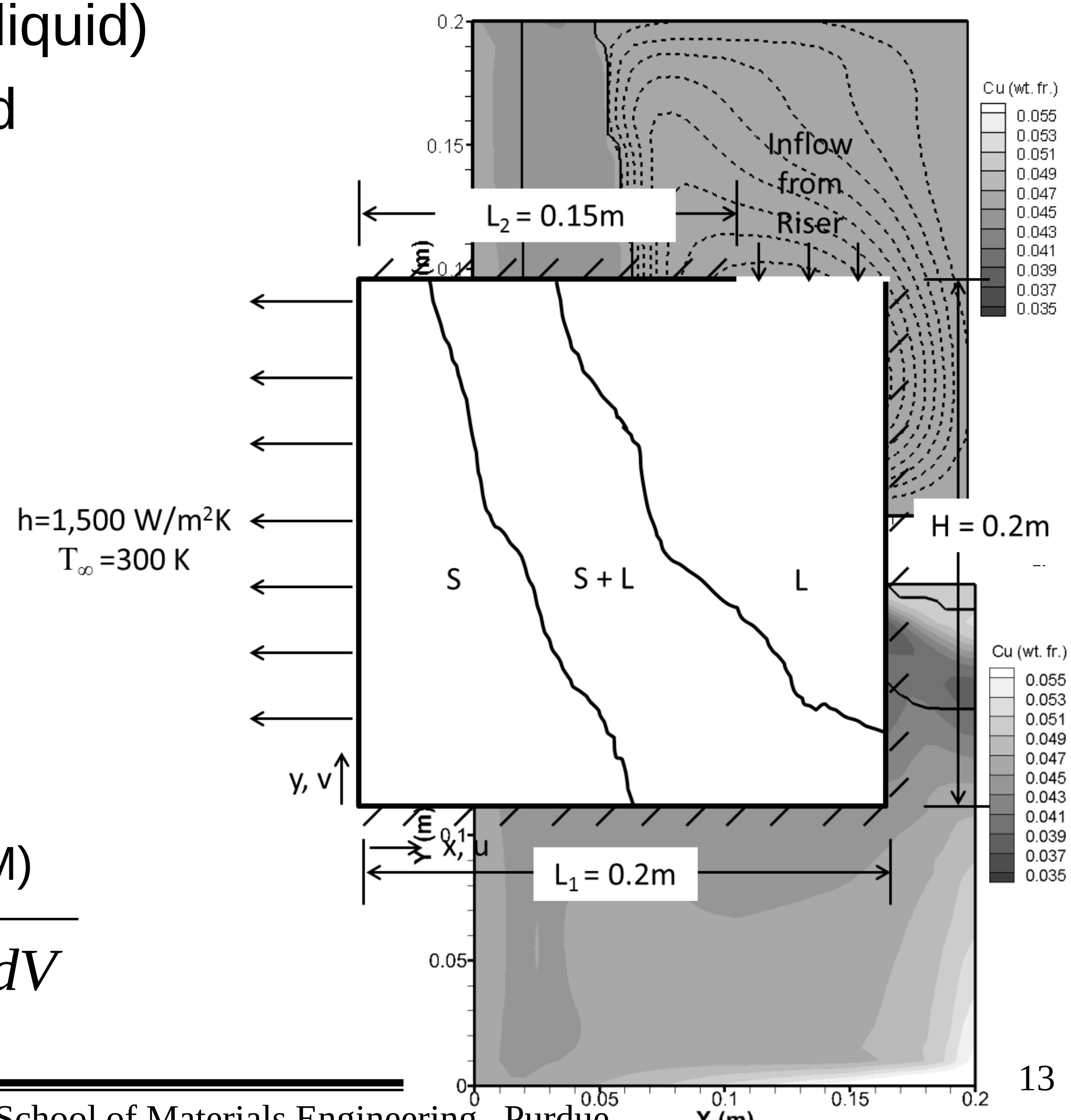
Application to static casting of Al-5wt% Cu

- Rigid mushy zone (solid + liquid)
- Solidification shrinkage and buoyancy drive liquid flow

- Uncertain inputs:
  - Dendrite arm spacing
  - Heat transfer coefficient
  - Material properties

- Outputs of interest:
  - Solidification time (t_s)
  - Macrosegregation number (M)

$$M = \sqrt{(1/V)\iiint (C/C_o - 1)^2\, dV}$$



Mixture transport model for alloy solidification

Conservation of mass:

$$\frac{\partial}{\partial t}(\rho)+\nabla\bullet\left(\rho\bar{V}\right)=0$$

Shrinkage

$\rho = \rho_S\, g_S + \rho_L\, g_L$

X-momentum:

Buoyancy Force

$$\frac{\partial}{\partial t}(\rho u)+\nabla\bullet\left(\rho\bar{V}u\right)=\nabla\bullet(\mu\nabla u)-\frac{\partial P}{\partial z}-\frac{\mu}{K}u+g\rho\left[\beta_T\left(T-T_0\right)+\sum\beta_C^i\left(C^i-C_0^i\right)\right]$$

Y-momentum:

$$\frac{\partial}{\partial t}(\rho v)+\nabla\bullet\left(\rho\bar{V}v\right)=\nabla\bullet(\mu\nabla v)-\frac{\partial P}{\partial r}-\frac{\mu}{K}v-\mu\frac{v}{r^2}$$

Drag Force $K \sim \lambda^2$

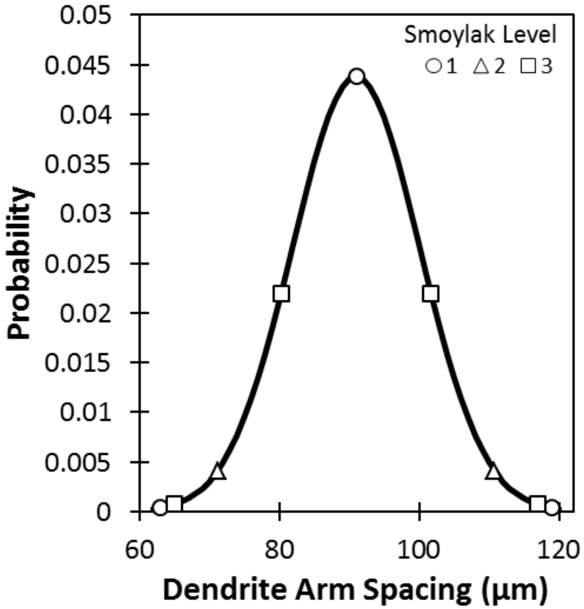
Species transport:

$$\frac{\partial\rho C^i}{\partial t}+\nabla\bullet\left(\rho VC^i\right)=\nabla\bullet\rho f_l D_l^i\nabla C^i+\nabla\bullet\rho f_l D_l^i\nabla\left(C_l^i-C^i\right)-\nabla\bullet\left(f_s\rho\left(V-V_s\right)\left(C_l^i-C_s^i\right)\right)$$

Energy transport:

$$\frac{\partial}{\partial t}\left(\rho c_p T\right)+\nabla\bullet\left(\rho c_p T\vec{V}\right)=\nabla\bullet(k\nabla T)-\frac{\partial}{\partial t}\left(\rho f_l L_f\right)-\nabla\bullet\left(\rho f_l L_f\vec{V}\right)-\nabla\bullet\left\{\rho f_s\left[\left(c_{pl}-c_{ps}\right)\; T+L_f\right]\;\left[\bar{V}-V_s\right]\right\}$$

Uncertainty in dendrite arm spacing



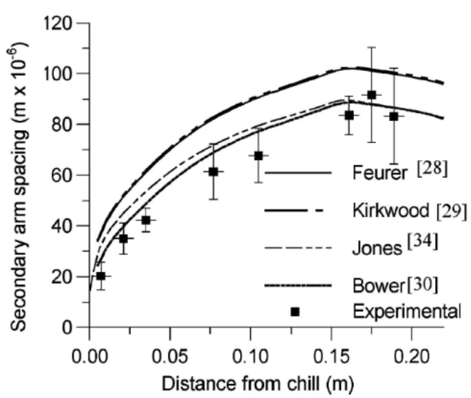


Figure 8 Variations in secondary spacing for different models Bower [28] and Jones [32] Feurer [26] and Kirkwood [27] compared to the experimental data for the directionally solidified Al 4.5 wt% Cu alloy.

- Begin with one input parameter, SDAS (λ)
- Flow in the mushy zone is damped by the drag on dendrite arms
- Blake-Cozeny model for permeability:

$$K = \frac{\lambda^2 g_l^3}{180 g_s^2}$$

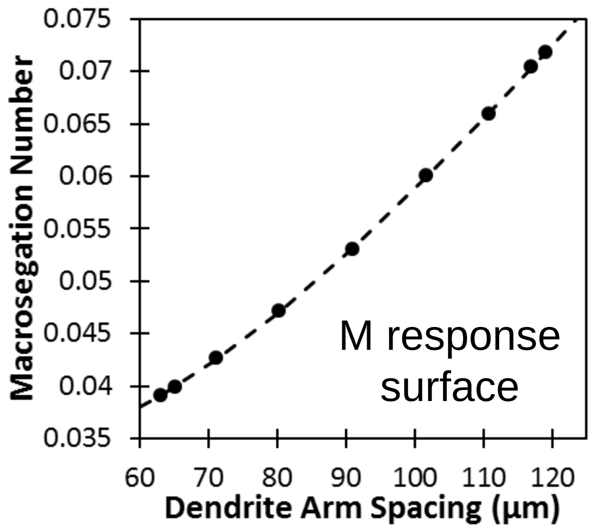
- Experimental measurements used as model inputs, including uncertainty
- Uncertainty captures variation within the part and measurement uncertainties

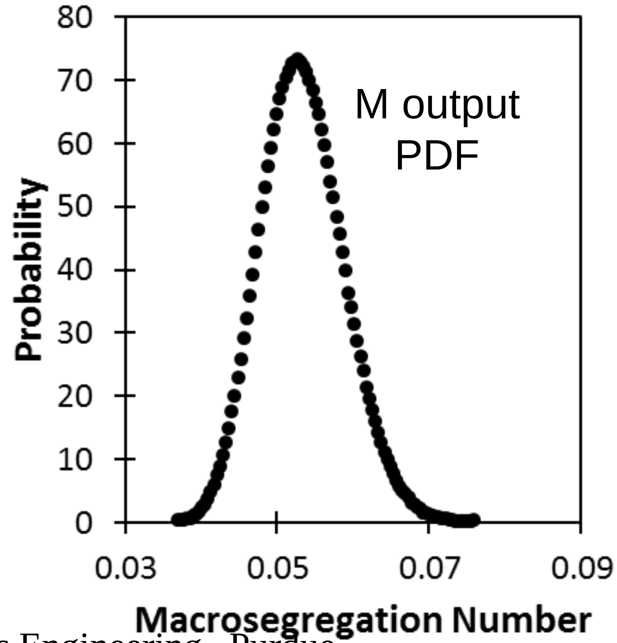
Data from Melo et al., *J. Mater. Sci.*, 2005

Effect of dendrite arm spacing uncertainty

- Solidification time is relatively unaffected by the uncertainty in arm spacing, as flow in mushy zone has little influence.
- For t_S: $\mu_o = 1410$ s, $\sigma_o = 2.3$ s, $2\sigma_o/\mu_o = 0.16\%$

- Macrosegregation increases with arm spacing
- For M: $\mu_o = 0.0534$, $\sigma_o = 0.00543$, $2\sigma_o/\mu_o = 20\%$

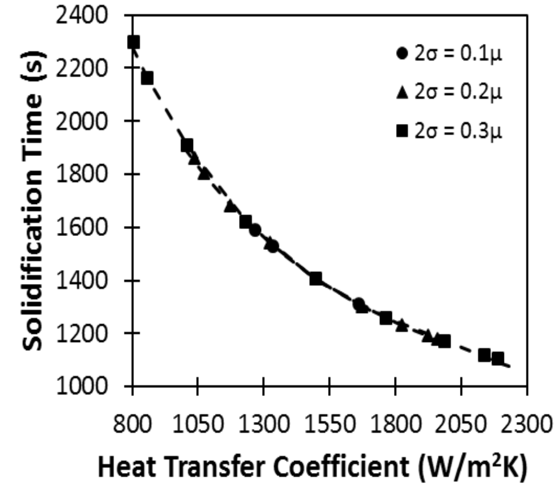




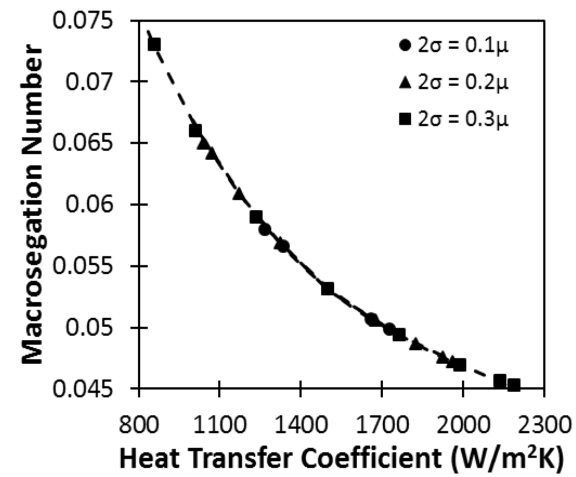
Uncertainty in heat transfer boundary condition

- Another sngle input case
- Thermal boundary conditions are difficult to measure
- Frequently, experimental correlations are published without uncertainty information
- Three different input distributions were considered
  - σ = 450 W/m^{2}K (30%μ)
  - σ = 300 W/m^{2}K (20%μ)
  - σ = 150 W/m^{2}K (10%μ)

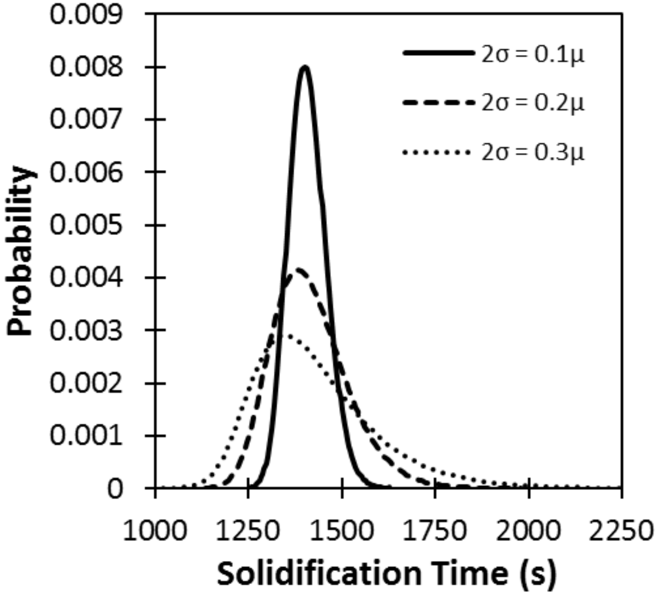
t_S response surface



M response surface



Effect of heat transfer coefficient uncertainty: Solidification time

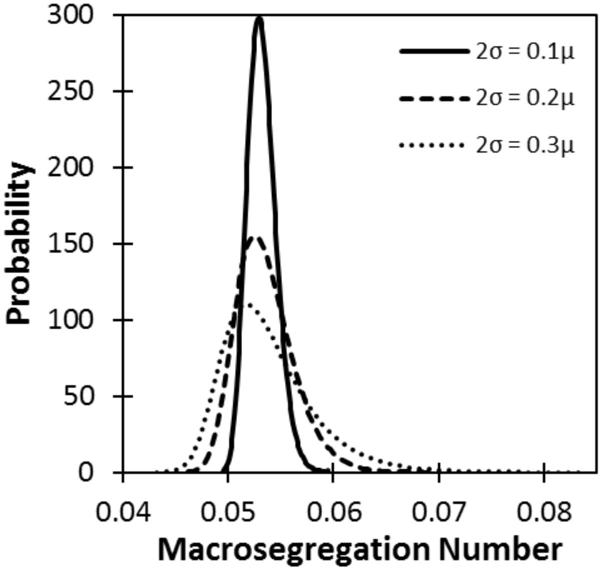


h σ_i	ts σ_o
2σ = 30% μ	2σ = 23.2% μ
2σ = 20% μ	2σ = 14.5% μ
2σ = 10% μ	2σ = 7.2% μ

The output uncertainty is lower than the input uncertainties

Boundary conditions need to be known better than 10% to have a solidification time prediction within 5%

Effect of heat transfer coefficient uncertainty: Macrosegregation



h σ_i	M σ_o
2σ = 30% μ	2σ = 16.2% μ
2σ = 20% μ	2σ = 10.4% μ
2σ = 10% μ	2σ = 5.2% μ

Slower heat transfer leads to larger mushy zones and more buoyancy driven macrosegregation

Wider range of mushy zones allows more flow at the low *h* side of PDF and less at high *h*; skews PDFs to low M

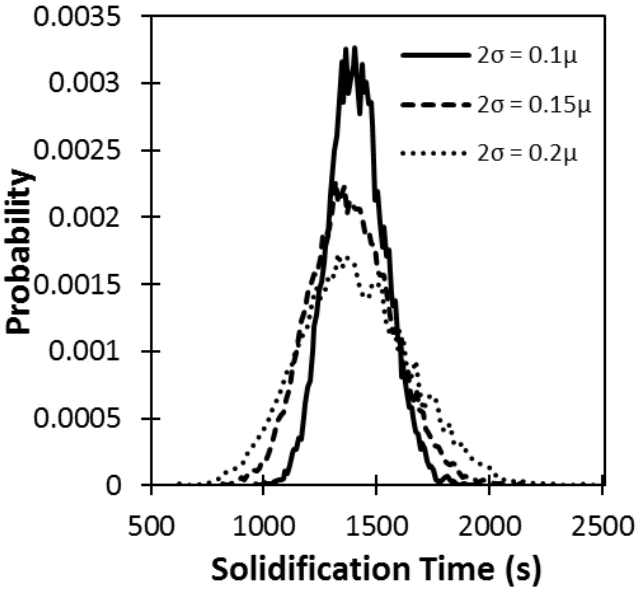
Uncertainty in multiple inputs: material properties

- Material property values are measured with some uncertainty (is it reported?)

- Three different levels of uncertainty in input distributions were analyzed:
  - $2\sigma = 20\%\ \mu$
  - $2\sigma = 15\%\ \mu$
  - $2\sigma = 10\%\ \mu$

ρ_s = 2750 kg/m^3
$\Delta\rho = \rho_l - \rho_s$ = -290 kg/m^3
k = 137.5 W/mK
c_p = 1006 J/kgK
L_f = 390000 J/kg

Effect of materials property uncertainty: Solidification time



Input σ_i	ts σ_o
2σ = 20% μ	2σ = 36% μ
2σ = 15% μ	2σ = 26% μ
2σ = 10% μ	2σ = 18% μ

- Uncertainties in these several input parameters combine to cause larger uncertainties in the solidification time than htc alone
- Large uncertainty in t_s even when the properties are known within 10%

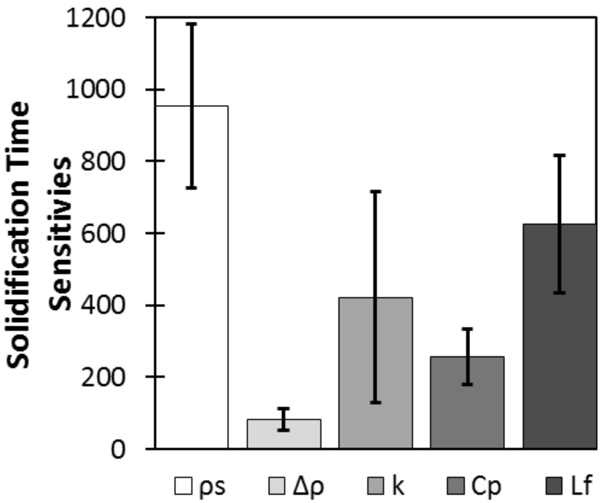
How do the individual properties affect t_s?

Sensitivity of solidification time to uncertainty in material properties

- "Sensitivity" is defined as

$$S_i \approx \overline{\frac{\partial \hat{f}}{\partial p_i}} \; (n\,\sigma_i)$$

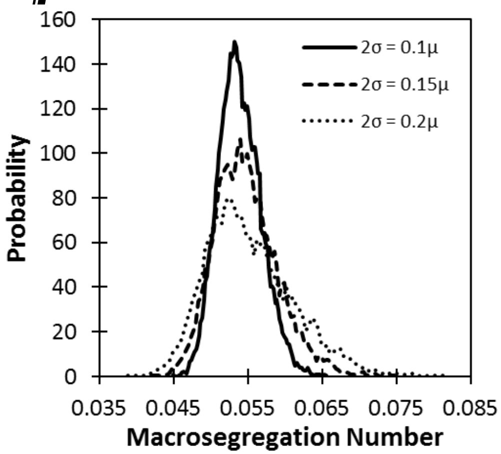
(complete definition in
Morris, *Technometrics*, 1991, and
Campolongo and Cariboni, *Env. Mod. Softw.*, 2007)

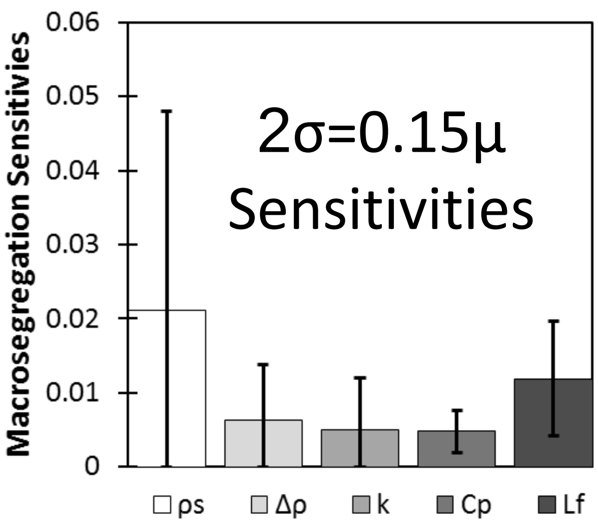


Sensitivities for 2σ=0.15μ case

- Density (and liquid density level) has largest effect on solidification time
- Density affects sensible and latent thermal capacity and fluid flow
- Shrinkage driven flow (through $\Delta\rho$) has the smallest effect on t_s
- Latent heat and thermal conductivity are also important

Sensitivity of macrosegregation to uncertainty in material properties



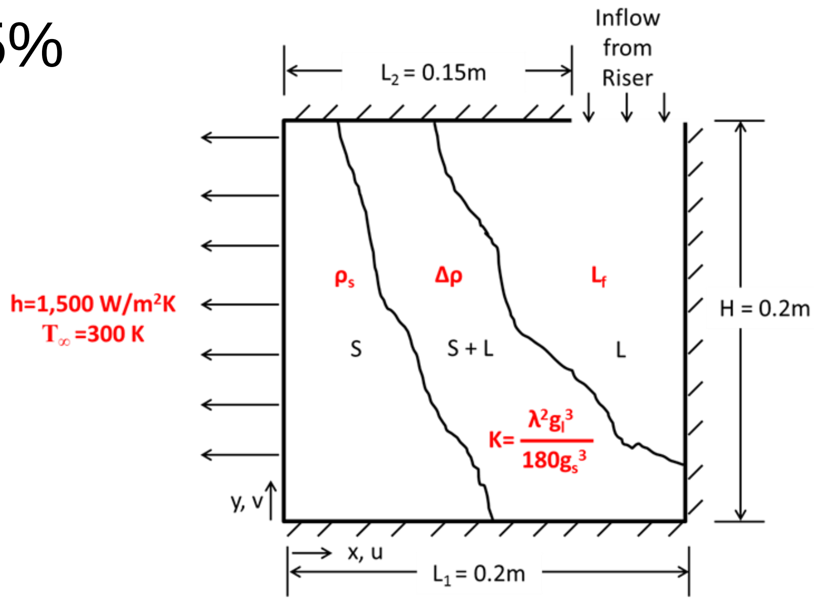


- *M* less sensitive than t_S to properties
- St $\approx$ 0.2 for this alloy (mushy zone thermal capacity and thickness dominated by latent heat)
- Macrosegregation is most sensitive to density (inertia, thermal capacity) and latent heat (thermal capacity)
- *M* is more tolerant of uncertainty in *k*, c_p, and solidification shrinkage

Input σ_i	M σ_o
2σ = 20% μ	2σ = 22% μ
2σ = 15% μ	2σ = 15.6% μ
2σ = 10% μ	2σ = 10.6% μ

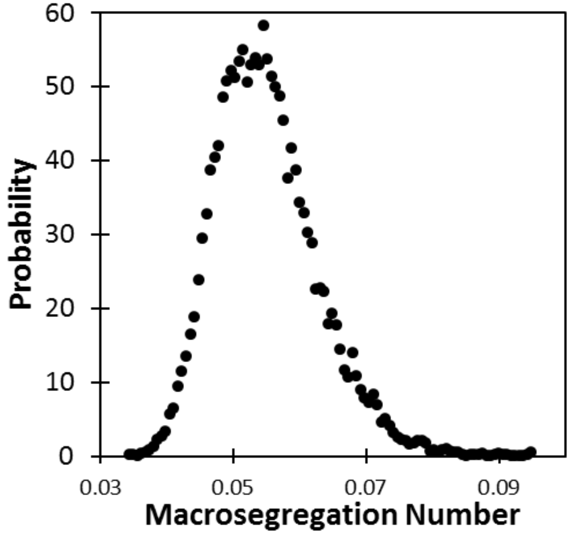
Effect on macrosegregation of uncertainty in material properties, heat transfer rate, and dendrite arm spacing

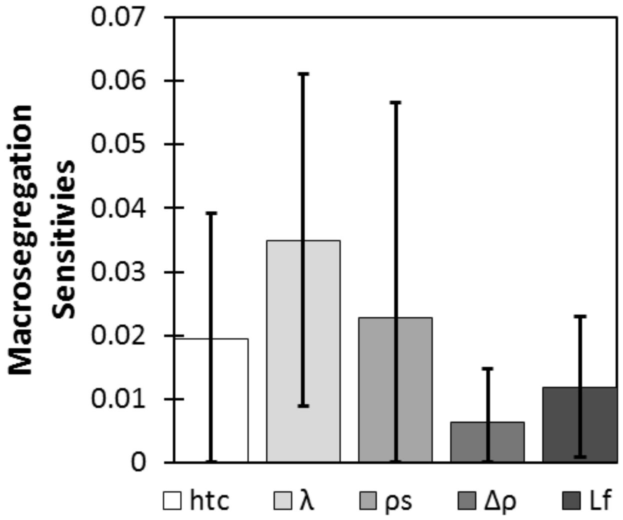
- Heat transfer, material property, and λ uncertainties analyzed together for *M*
- Dendrite arm spacing: 2σ = 15%
- Material properties: 2σ = 15%
- Heat transfer: 2σ = 20%



k and c_p had the least influence on M and were neglected here

Macrosegregation Uncertainty and Sensitivity





- Mean $M = 0.055$
- 2σ of $M = 0.0076$ (14%)

- M has the largest average sensitivity to λ (controls flow)
- Heat transfer coefficient and density are next largest

- M has the smallest average sensitivity to solidification shrinkage

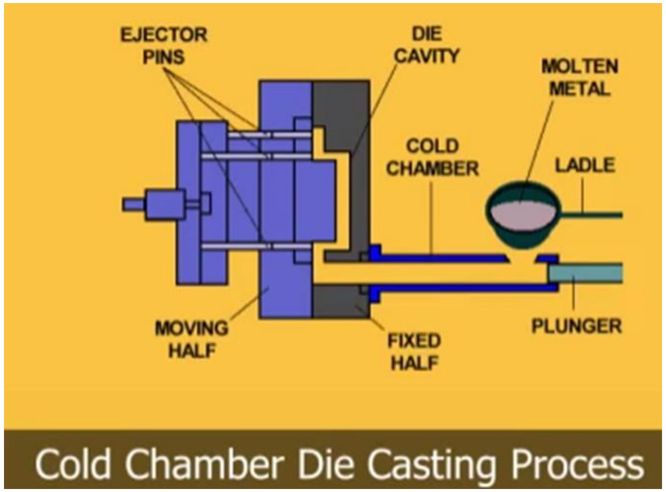
Observations from application to static casting

- M and t_s most sensitive to density, perhaps easiest property to measure with low uncertainty
- Ranking of sensitivity depends on output of interest
  (e.g., λ important to M but not t_S)
- Perhaps it is easier to reduce uncertainties in measurement of properties than, say λ or h – pick low-hanging fruit that has impact
- This type of analysis can help us answer Dr. Quested's question: what is the payoff to driving the uncertainty in property values lower? (and which property values?)
- But, how do we obtain the uncertainties of the inputs? Is that information available?

A commercial application: Modeling High Pressure Die Casting

Use UQ process on application in real industrial setting

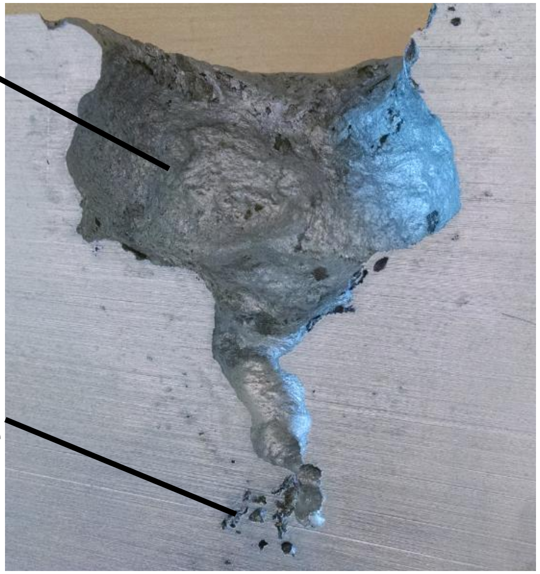
- High pressure die casting of aluminum part for car transmission
- Use commercial software for process modeling (license)



North American Die Casting Association (NADCA)

External shrinkage

Internal shrinkage



Outputs of Interest:

- Location and extent of porosity
- Solidification time

Work sponsored by Fiat-Chrysler Automotive, Kokomo Casting Plant, Indiana, USA

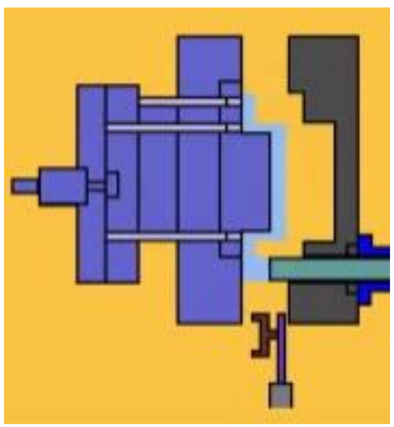
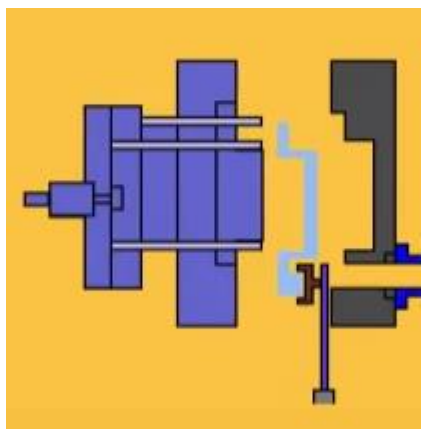
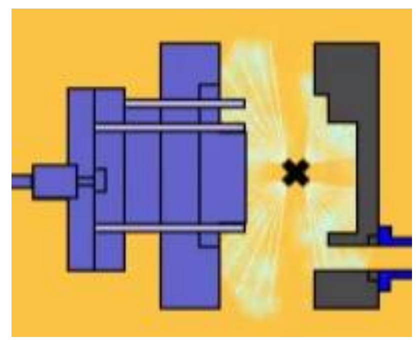
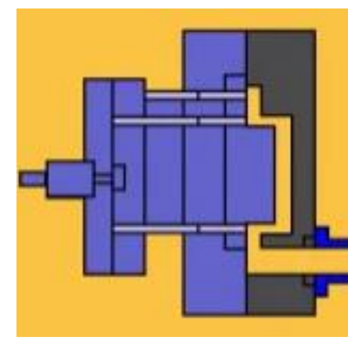
High Pressure Die Casting Process

Casting cycle:

Die Close & Solidification — 20s

Die Open & Delay Time

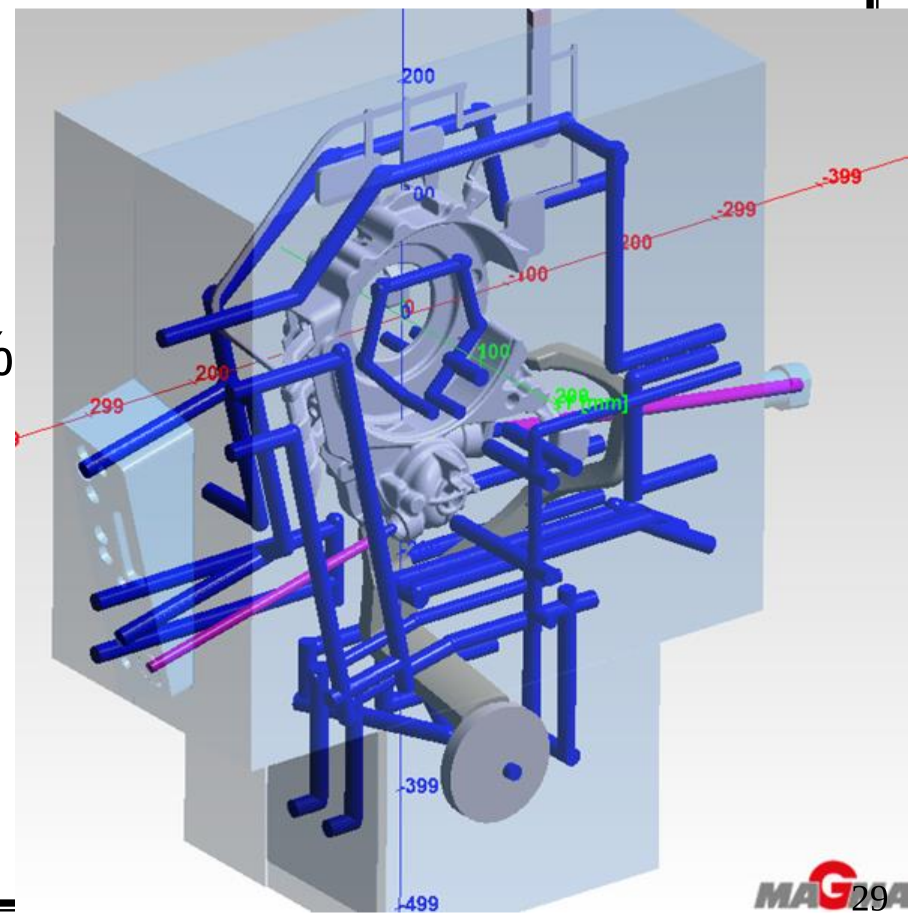
Metal Filling — *Cover Die remove* — *Casting ejected* — Lubricate — Air Blowing — *Die Close* — *Metal Filling*

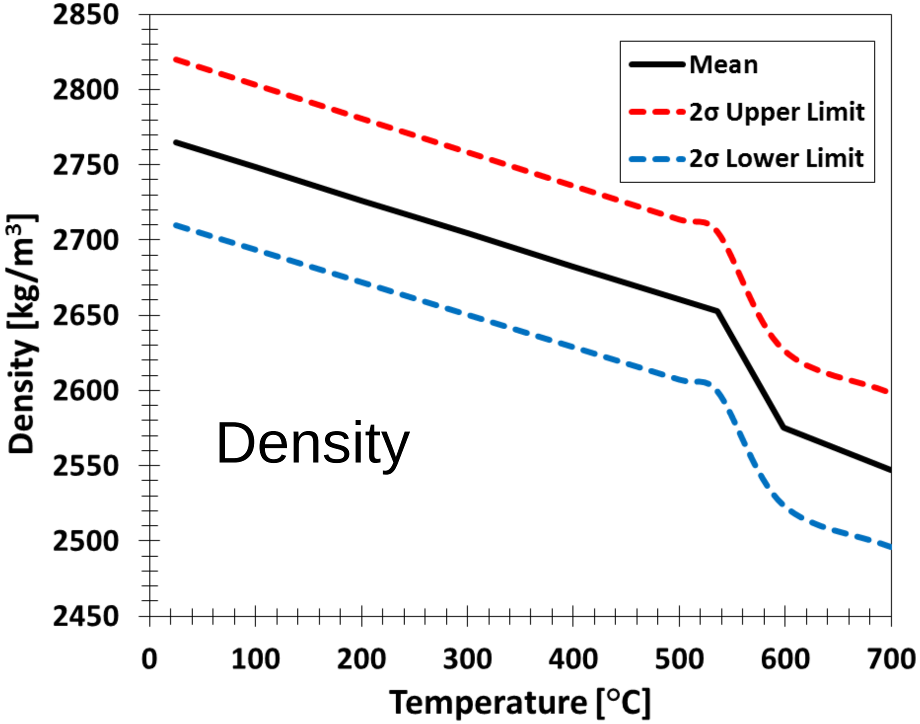
North American Die Casting Association (NADCA)

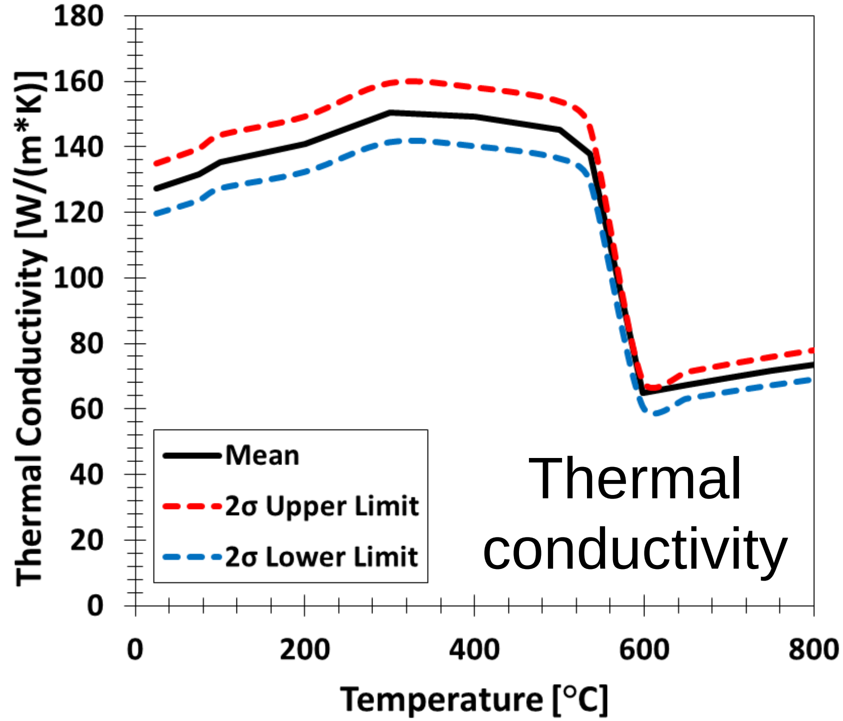
Simulation of HPDC Process

- Commercial software: MAGMA
- 9 Heating Cycles +
  1 “Production” Cycle
- A380 part, H13 steel mold
- Initial Al temperature = 643 ℃
- Initial die temperature = 25 ℃
- Default Feeding Effectivity: 30%
- No filling process simulation
- No fluid flow
- Types of uncertainty:
  - Material properties
  - Boundary conditions



Property uncertainty: density and thermal conductivity





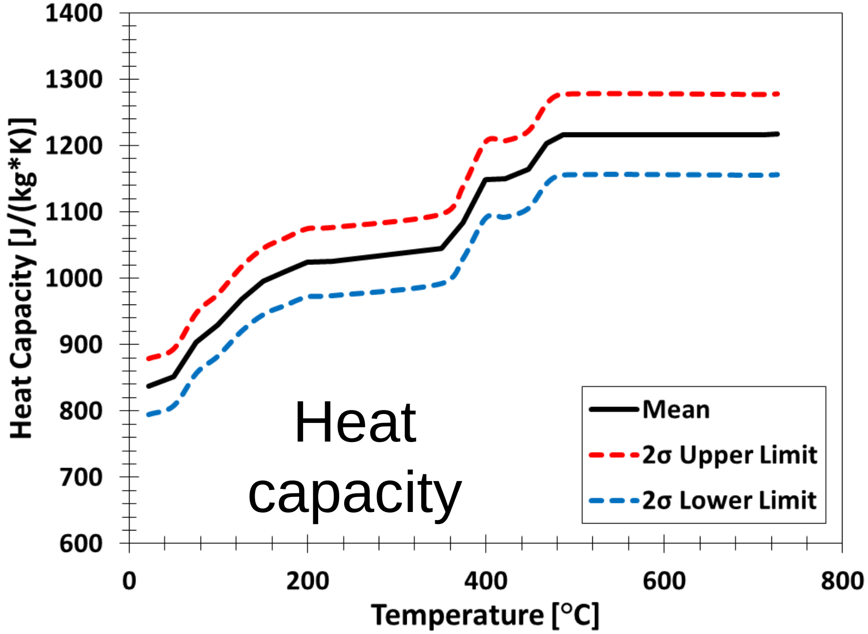
Experimental uncertainty of $\pm$2%

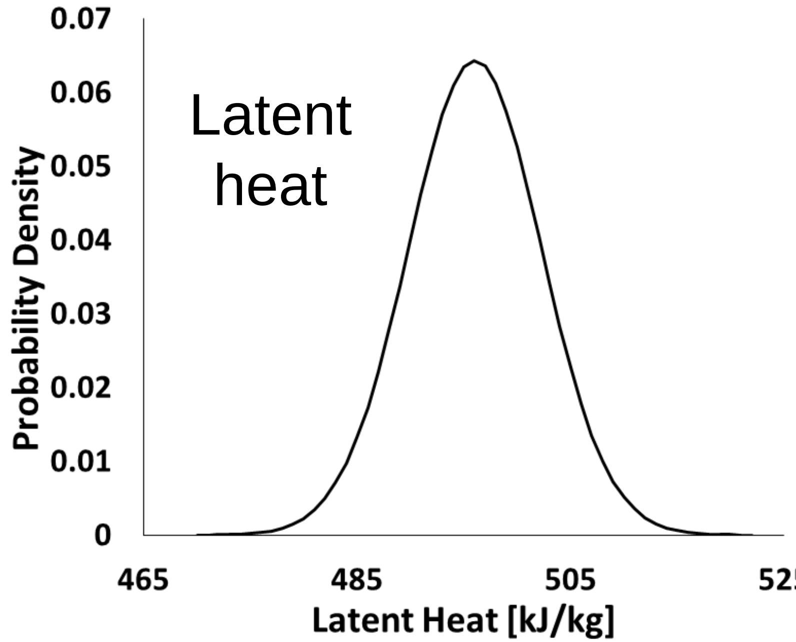
Overfelt et al., *High Temp.-High Pressures,* 2002

Experimental uncertainty of $\pm$6%

Brandt et al., *Int. J. Thermophysics,* 2007

Property uncertainty: heat capacity and latent heat





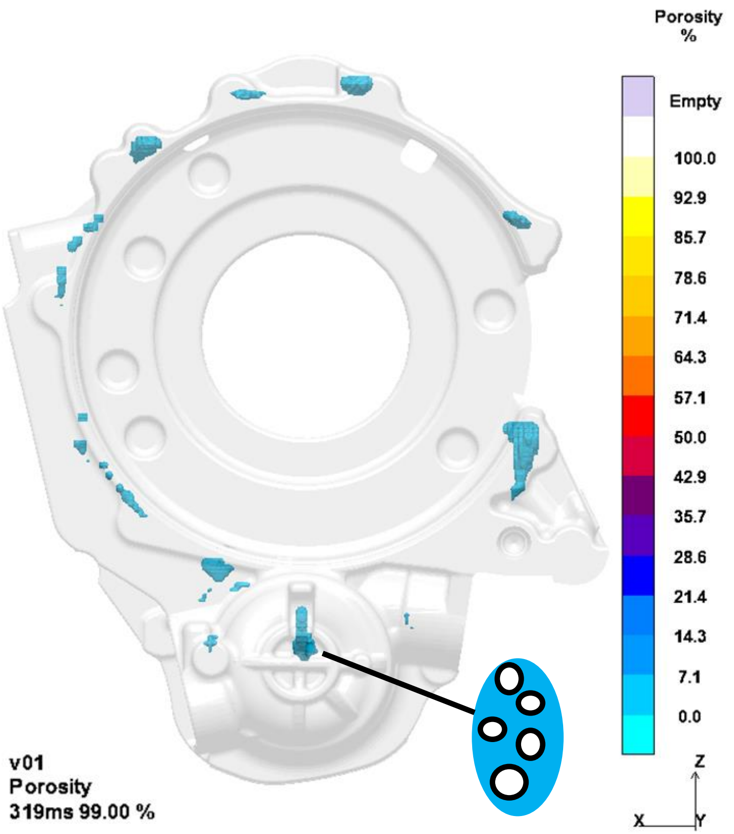
- Data for A380 not available
- Used data for A319 (similar composition)
- Experimental uncertainty of $\pm$5%

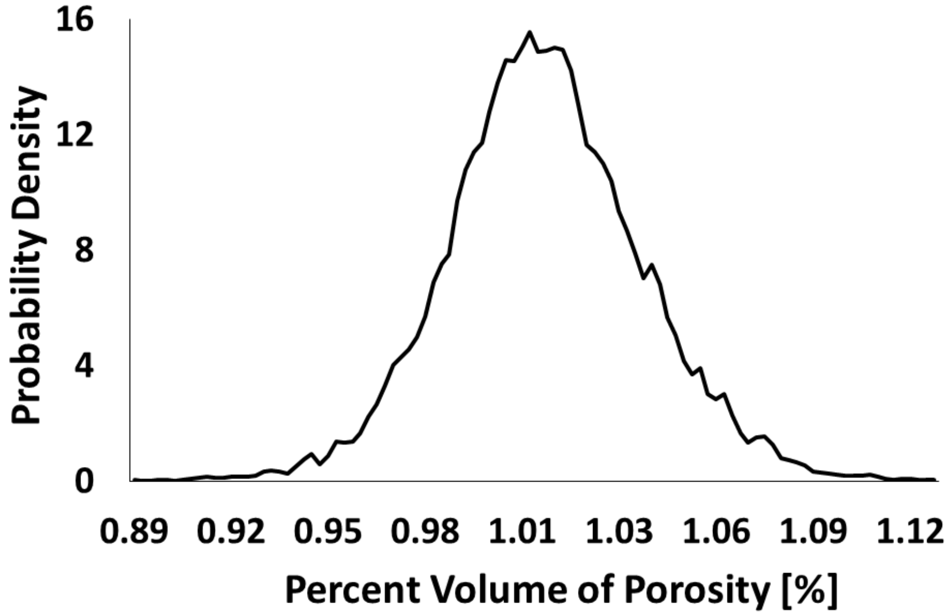
Rudtsch, *Thermochimica Acta,* 2002

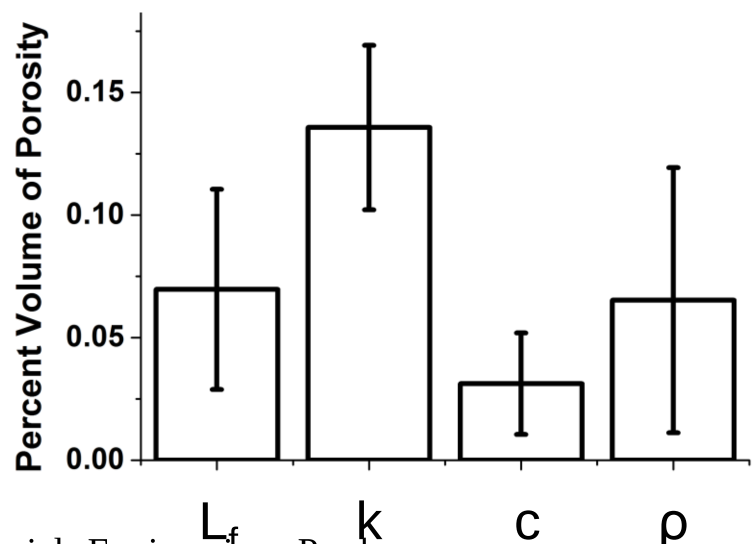
Experimental uncertainty of $\pm$2.5%

Đurđević et al, *Metalurgija,* 2003

Uncertainty in Porosity due to property uncertainty

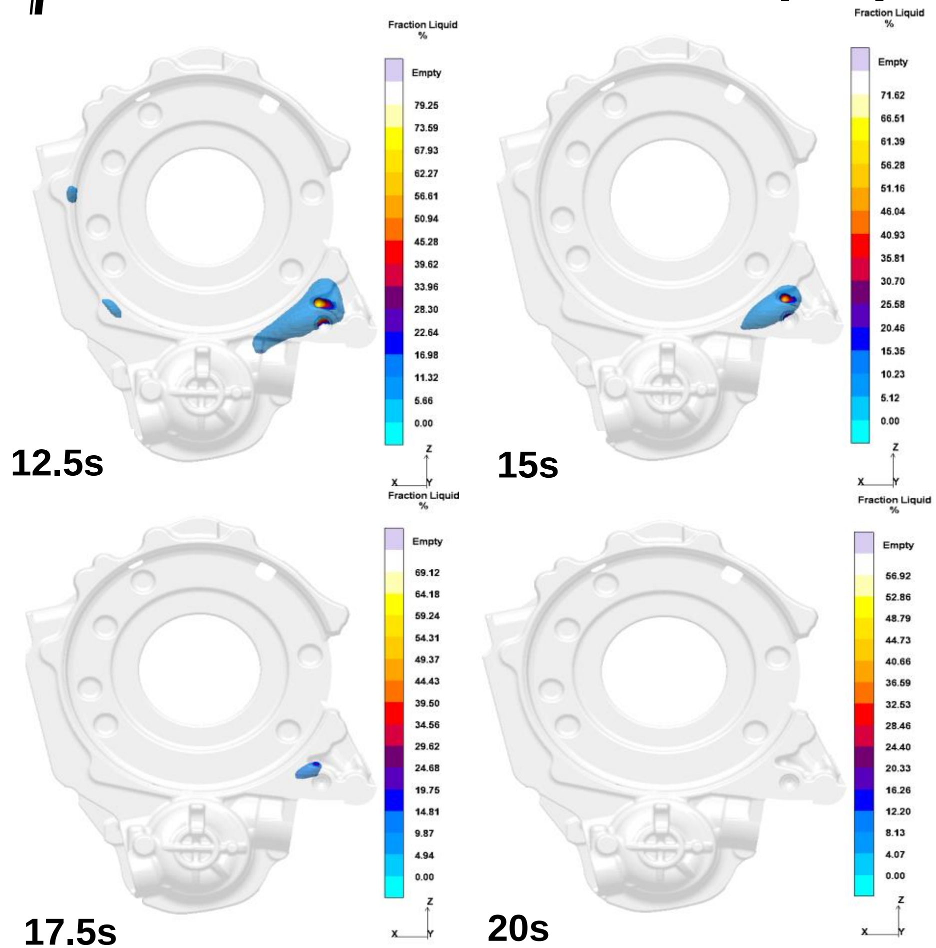


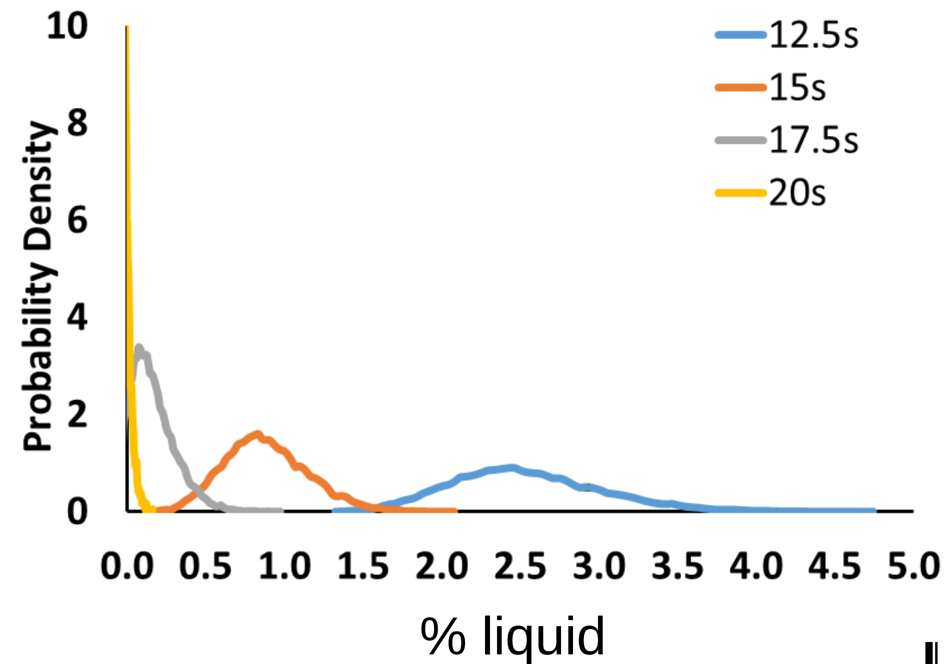




- $\mu = 1.01\%$, $\sigma = 0.03\%$, $2\sigma/\mu = 5.9\%$
- Small effect on porosity predictions

Uncertainty in fraction liquid remaining due to property uncertainty

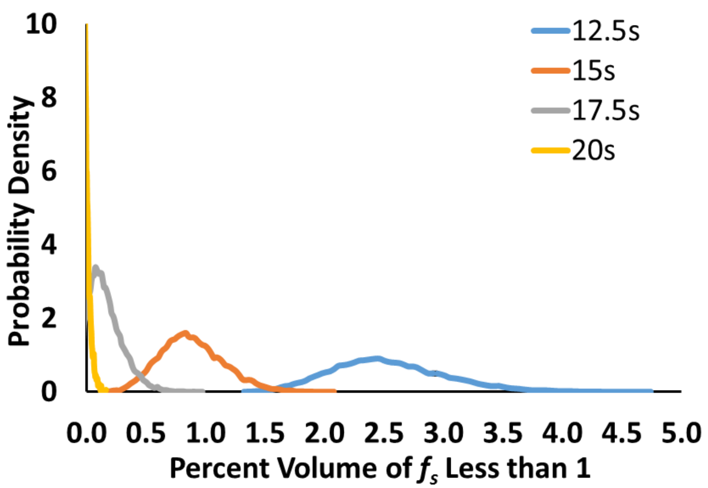


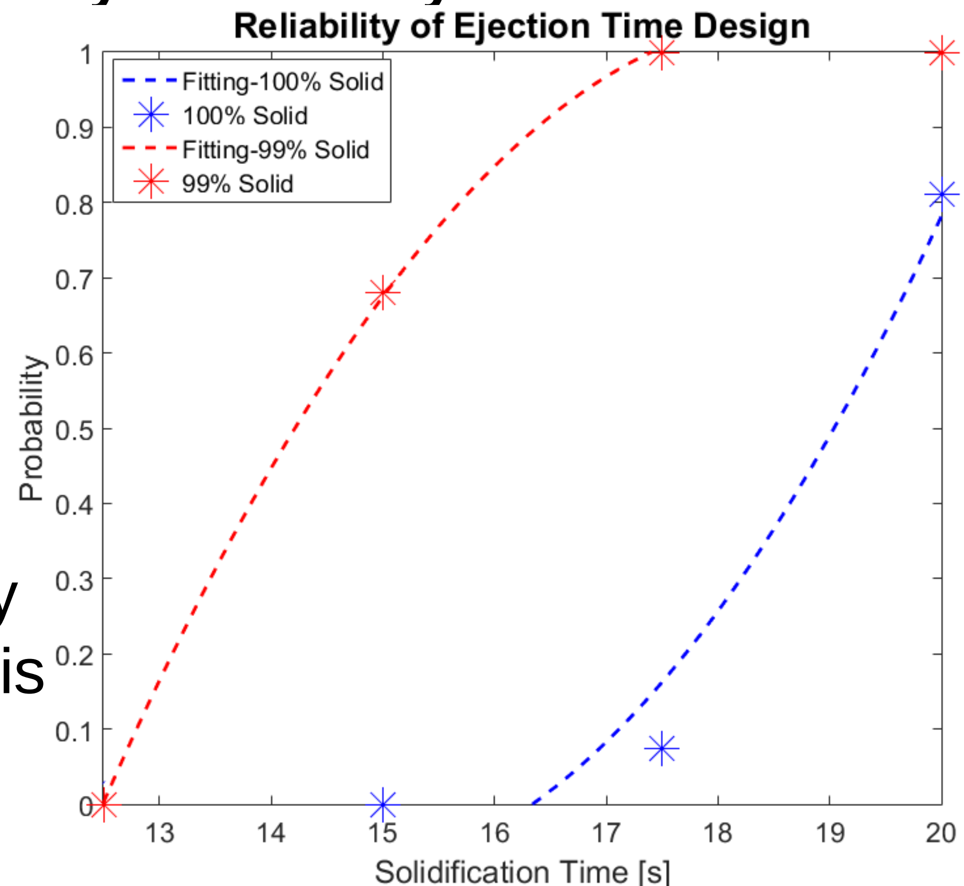


What is probability that there is liquid left at ejection time?

Colored regions are volumes not fully solid

Uncertainty in fraction liquid remaining due to property uncertainty

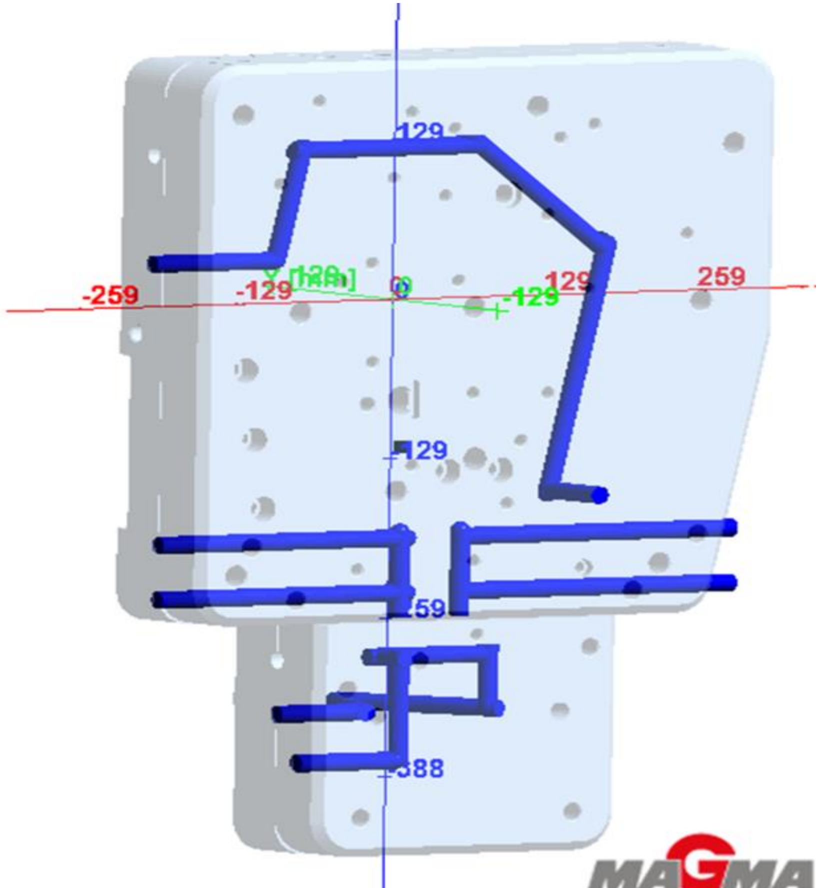




Cannot ensure casting fully solid at 20 s, but 99% solid is possible

Current process reasonable, with no one property dominating output uncertainty

Uncertainty in Cooling Conditions: straight tubes



Dittus-Boelter equation

$$Nu_D = 0.023 Re_D^{0.8} Pr^{0.3}$$

$$\begin{bmatrix} 0.6 \lesssim Pr \lesssim 160 \\ Re_D \gtrsim 10{,}000 \\ \frac{L}{D} \gtrsim 10 \end{bmatrix}$$

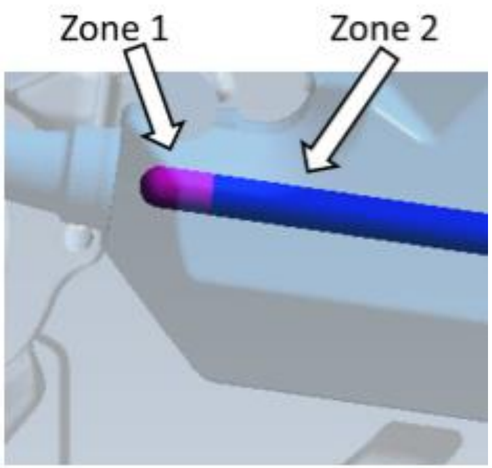
Under process conditions, heat transfer coefficient is (in W/m^2K):

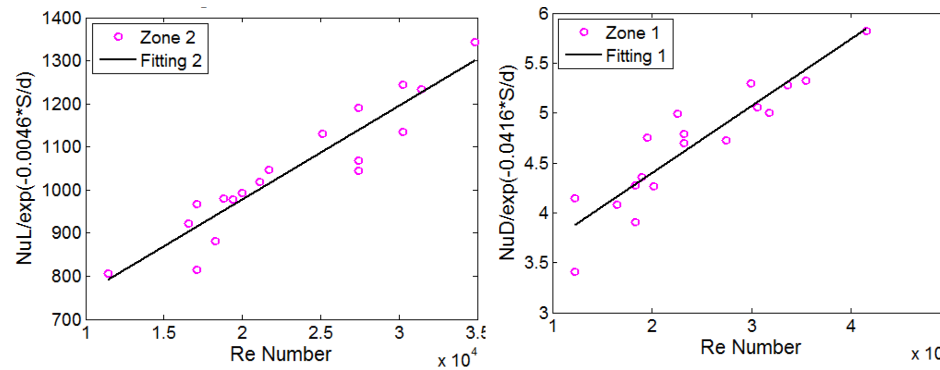
μ=8000, 2σ = 1600

(20% uncertainty)

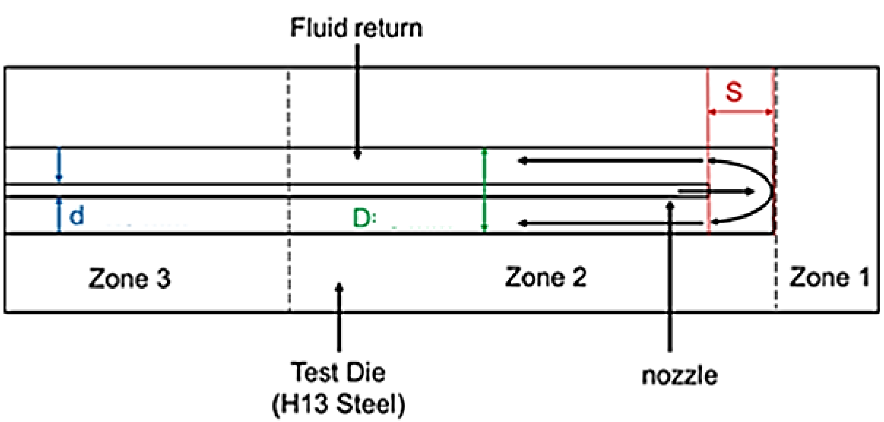
Jo et al., *Nuc. Eng.Tech., 2*014

Uncertainty in Cooling Conditions: cooling jets

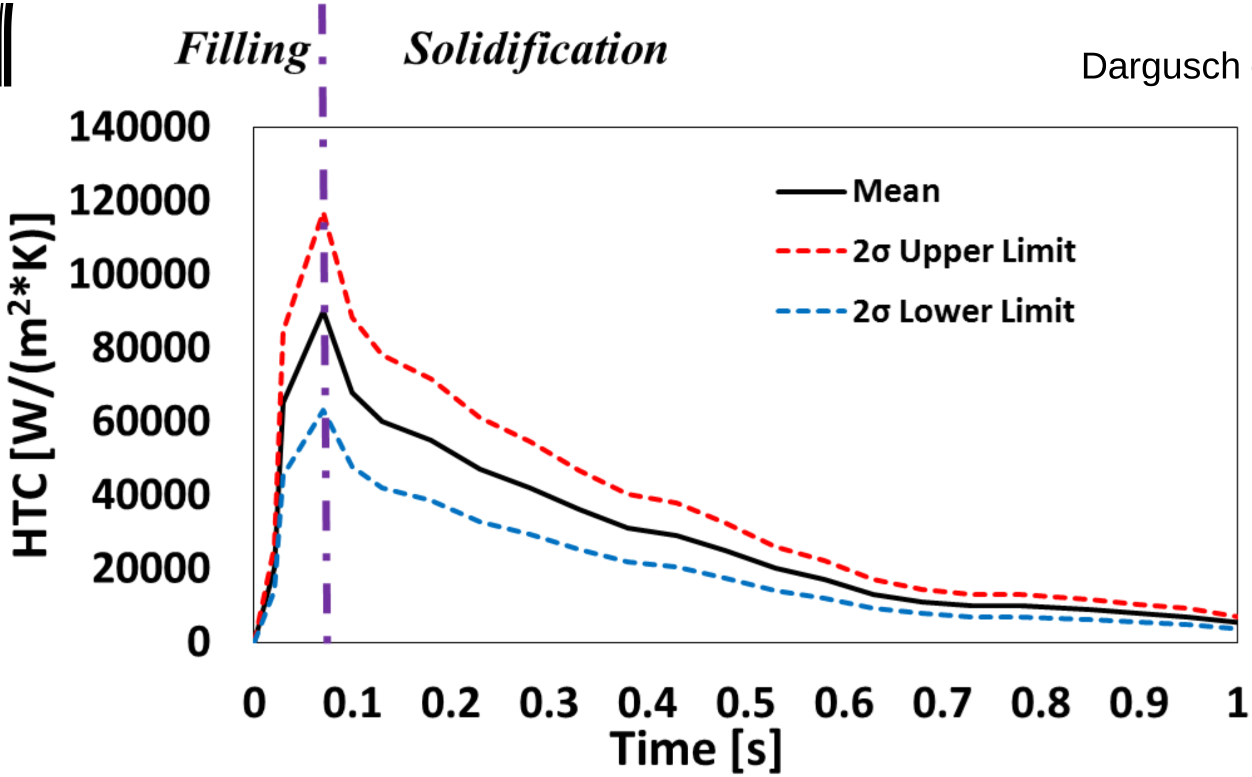




- Data fit to correlations for heat transfer coefficients as function of water flow rate
- Under process conditions, heat transfer coefficients are (in W/m^2K):
  - Zone 1: μ = 234.01, 2σ = 27.84
  - Zone 2: μ = 3509.18, 2σ = 427.8
  - 2σ/ μ ≈ 12% for both cases



Uncertainty in Cooling Conditions: metal-die interface



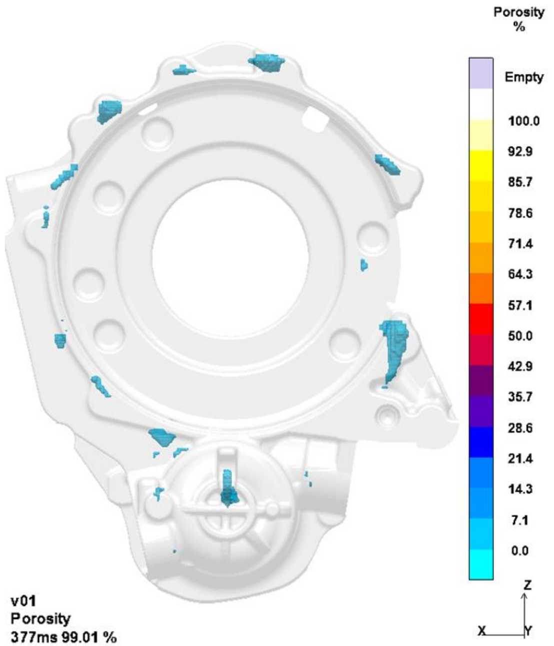
Dargusch et al, *Adv. Eng. Mater.*, 2007

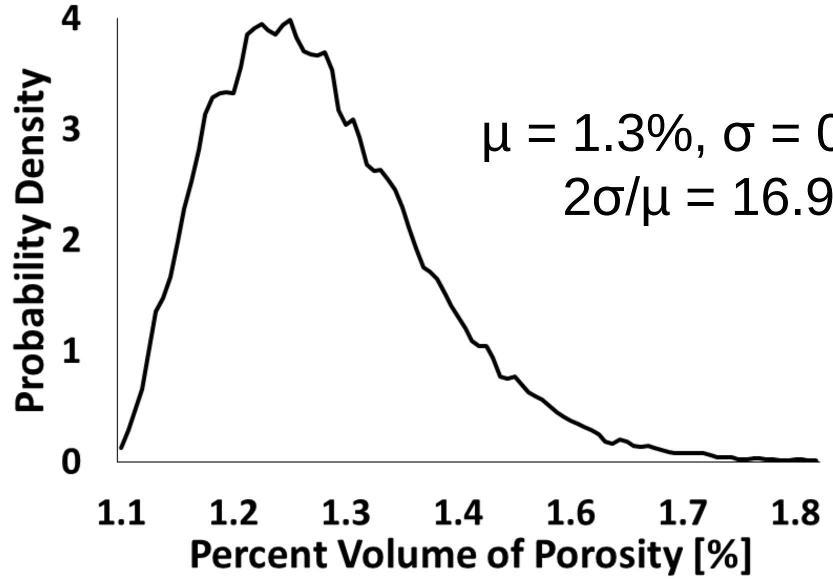
Experimental uncertainty of $\pm$30%

HTC is highest at end of filling, with pressure on liquid.

HTC decreases as shrinkage pulls metal from die.

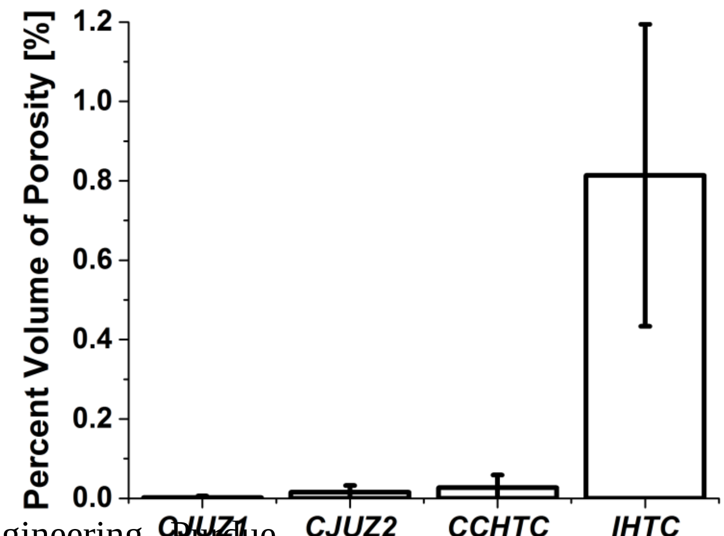
Uncertainty in Porosity due to HTC uncertainty



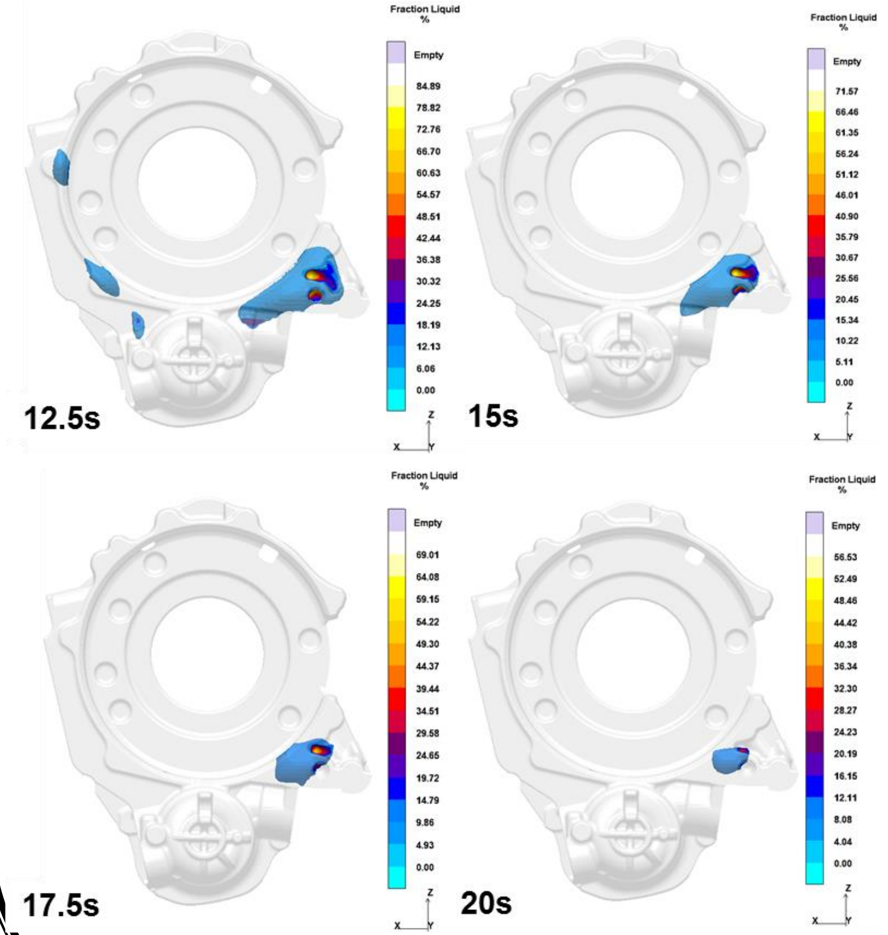


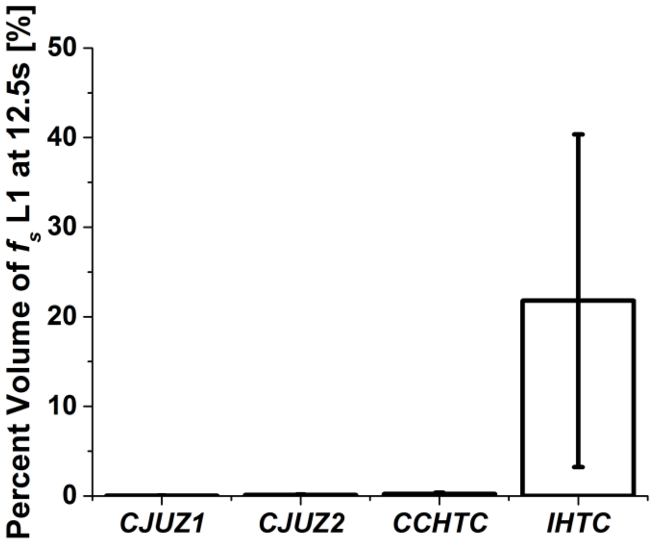
- Predicted porosity uncertainty is nearly 3 times larger than that due to material properties

- Only interfacial heat transfer has an effect on porosity development (dominant cooling mechanism)



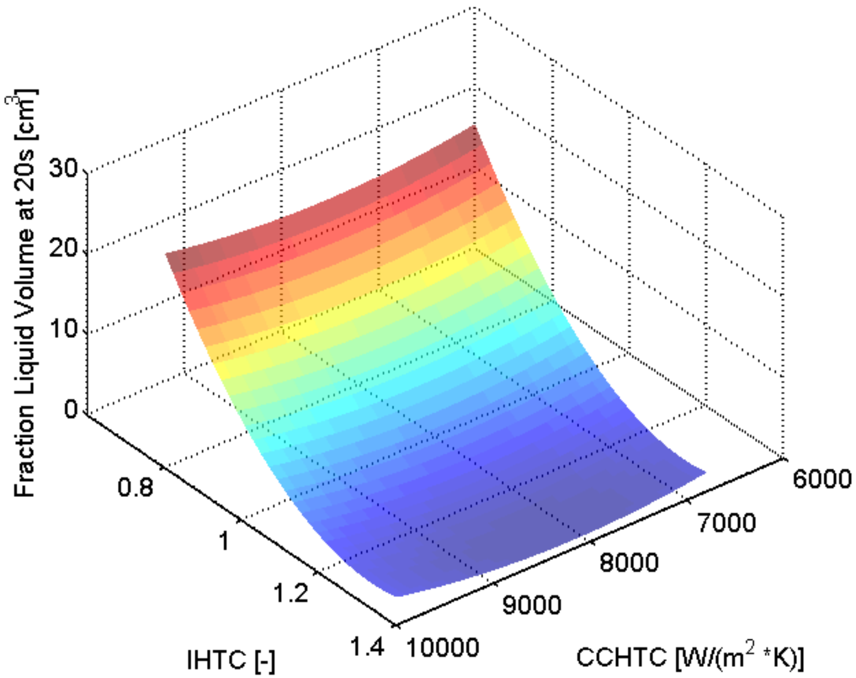
Sensitivity of fraction liquid remaining to HTC uncertainty



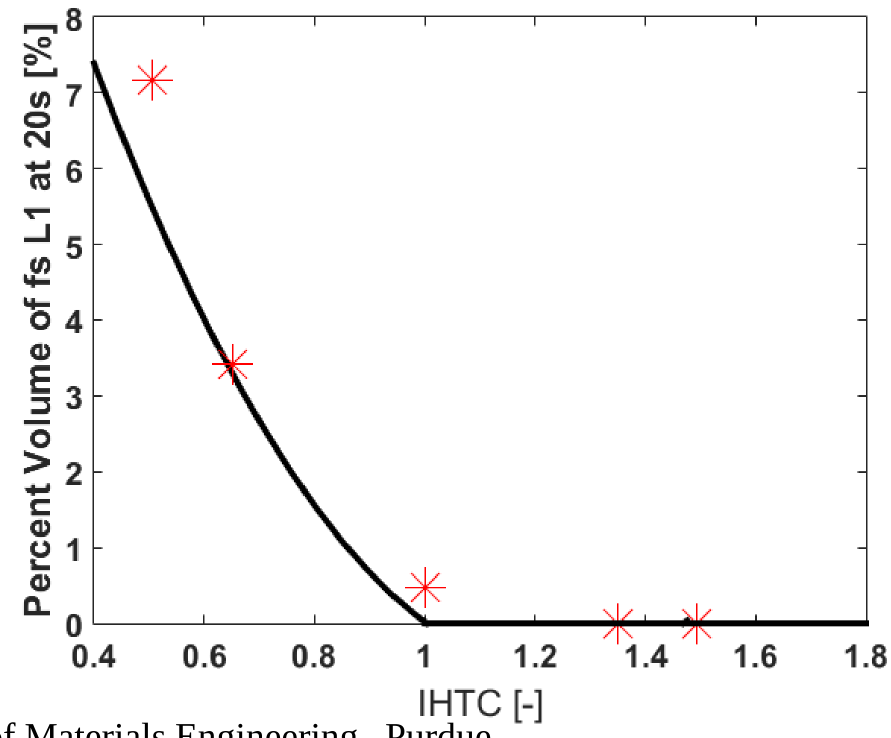


Fraction liquid results are most sensitive to uncertainty in interfacial heat transfer

Response surface for fraction liquid remaining due to HTC uncertainty

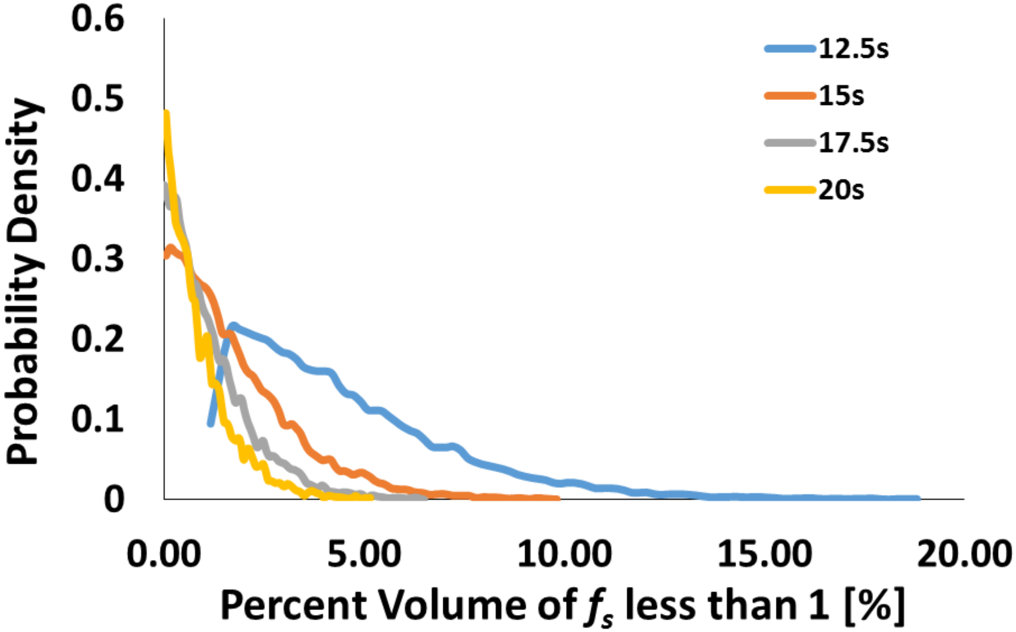


Use of polynomials for response surfaces can lead to nonphysical results (e.g., fraction liquids < 0)

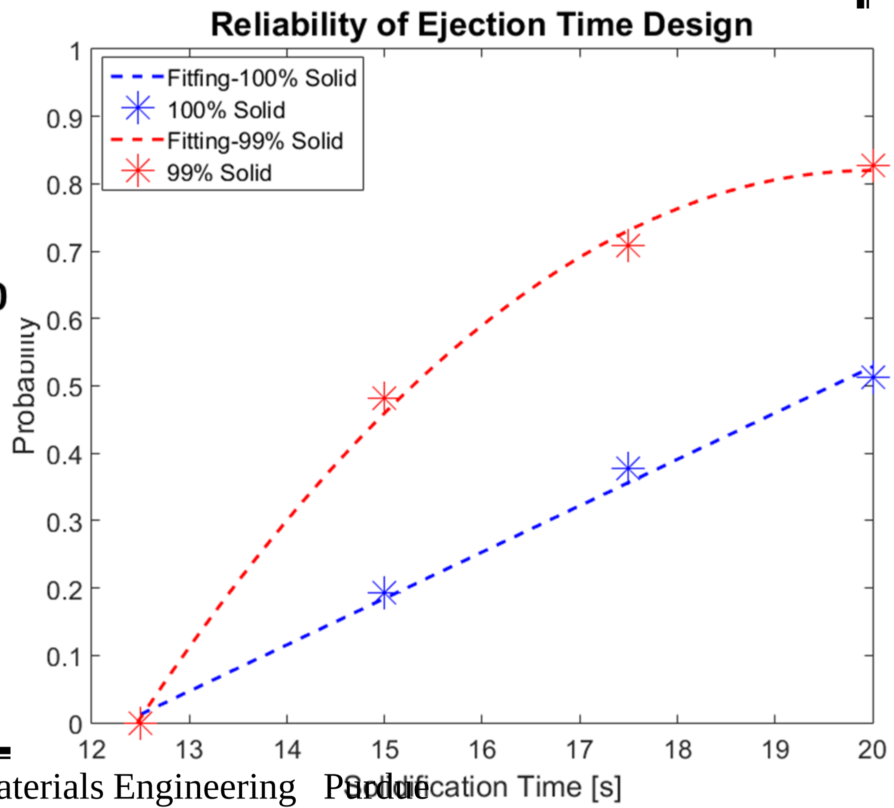


Need to correct surrogate model as a function of IHTC

Uncertainty in fraction liquid remaining due to HTC uncertainty



Uncertainty in interfacial heat transfer produces large uncertainty that all metal is solid at ejection



Current analysis suggests that the highest fraction solid with almost 100% certainty is ~98%

Observations from application to commercial HPDC process

- Ranked influence of material property and boundary condition uncertainty on PDFs of porosity and remaining liquid

- Most important factor is uncertainty in interfacial heat transfer
  - Uncertainty in other thermal conditions not critical for predicting outputs of interest
  - Material properties have only small influence

- Under current conditions, there is a probability that some liquid may remain at part ejection: Is this a problem?

- Can use UQ process in alterations of old or design of new processes

Recent and forthcoming articles on this topic

- K. Fezi and M.J.M. Krane, “Uncertainty Quantification in modeling equiaxed alloy solidification,” *International Journal of Cast Metal Research,* published online, 8/10/16.
- K. Fezi, M. J. M. Krane, "Uncertainty quantification in solidification modeling," in *Modeling of Casting, Welding and Advanced Solidification Processes - XIV*, H. Yasuda et al (eds.) IOP (2015).

- K. Fezi and M. J.M. Krane, “Uncertainty Quantification in modeling metal alloy solidification,” in review.
- A. Plotkowski and M.J.M. Krane, “Quantification of epistemic uncertainty in grain attachment models for equiaxed solidification,” in review.
- K. Fezi and M. J. M. Krane, “Uncertainty propagation in numerical modeling of aluminum direct chill casting,” in review.