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ASSESSMENT OF SURROGATE MODELING TECHNIQUES FOR USE IN 2D UNCERTAINTY QUANTIFICATION OF ABLATION HEAT TRANSFER

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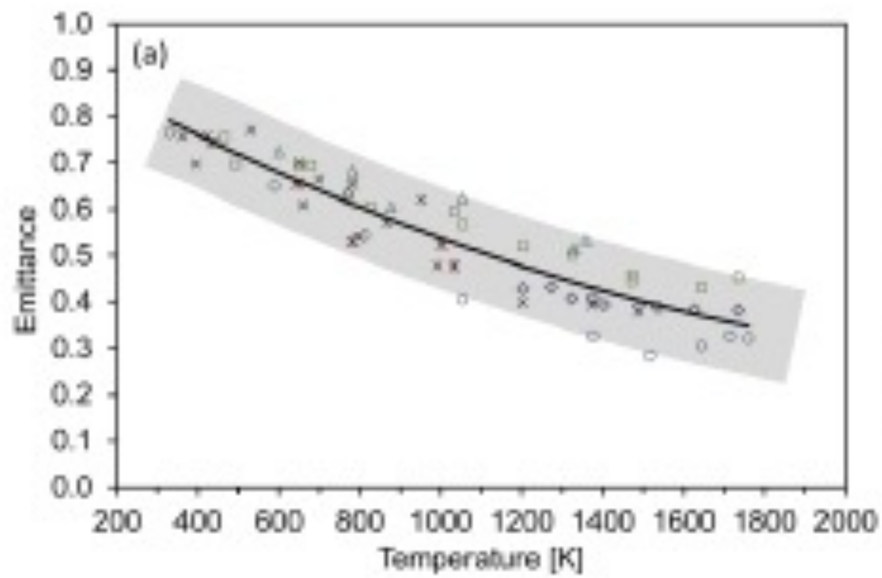
Outline

- What is a surrogate model?
- How do surrogate models apply to 2D Uncertainty Quantification?
- How do sensitivity studies support surrogate model generation?
- Case study
- Techniques used in case study.
- Computational cost and accuracy of different techniques.
- Conclusions
- References

What is a surrogate model?

- Surrogate models are analogous to a mathematical function that represents experimental data.
- Instead of a "fit" representing experimental data in figure to the right, the surrogate model represents the output that is otherwise generated by a computational model.
- A surrogate model estimates the output of a large, complex, computationally expensive model.
  - Surrogate model computes output much faster.
- A surrogate model is an estimate of computational model output and error may exist between surrogate model prediction and computational model prediction.
  - Surrogate model form error



Normal total emittance of aluminum oxide as a function of temperature.[1]

Surrogate model estimates the output of complex simulations more efficiently.

Application of surrogate models to 2D Uncertainty Quantification (2D-UQ)

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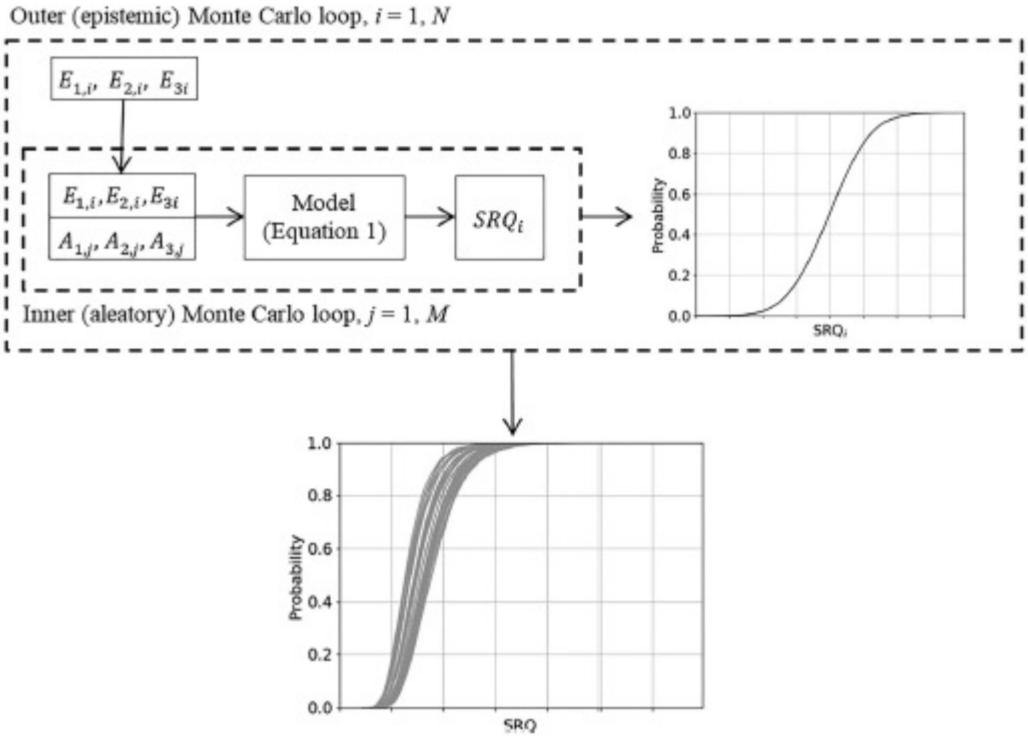
- Steps to perform a 2D-UQ[2]

1. Define the system response quantity (SRQ) or quantities.
2. Define the model.
   a. Mathematical model
   b. Geometrical model
3. Identify relevant inputs.
   a. Informed through engineering judgement and sensitivity analyses
4. Classify and characterize input uncertainties.
   a. Classified into aleatory and epistemic categories
5. **Propagate aleatory uncertainties in "inner loop".**
   a. Aleatory Loop
6. **Propagate epistemic uncertainties in "outer loop".**
   a. Epistemic Loop
7. Quantify the uncertainty.
   a. System Variability
   b. Model Credibility

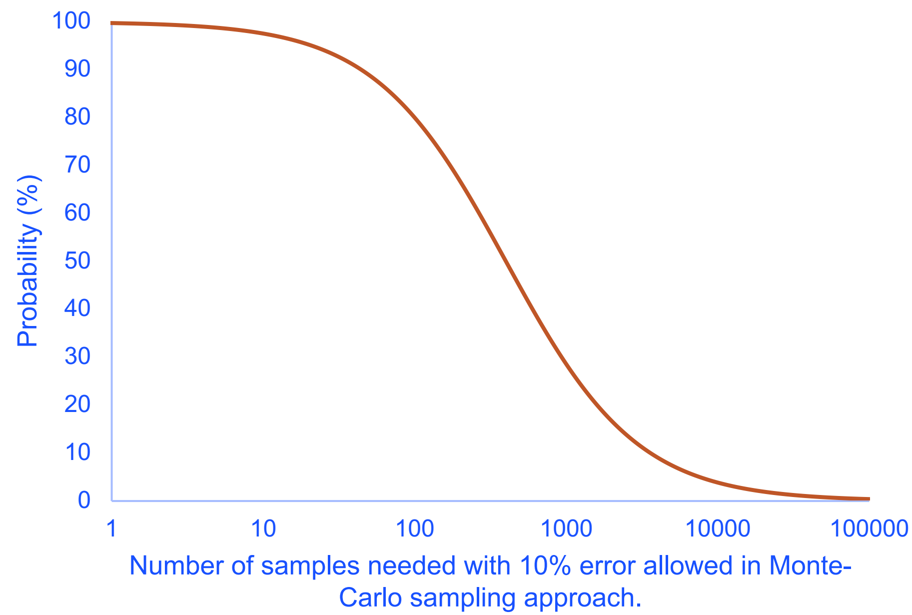


Two-dimensional Monte-Carlo Approach.[2]

Surrogate model is used in the propagation of aleatory and epistemic uncertainty.

Propagation of aleatory and epistemic uncertainty

- Several samples may be needed depending on number of inputs, accuracy desired, and probabilities of interest.
- Example: Want less than 50% probability with 10% error.
  - Need 400+ simulations
- Example: 1,000 aleatory samples and 500 epistemic samples.
  - Need 500,000 simulations
  - Computationally intractable for single processor and inefficient use computer resources if they are available.



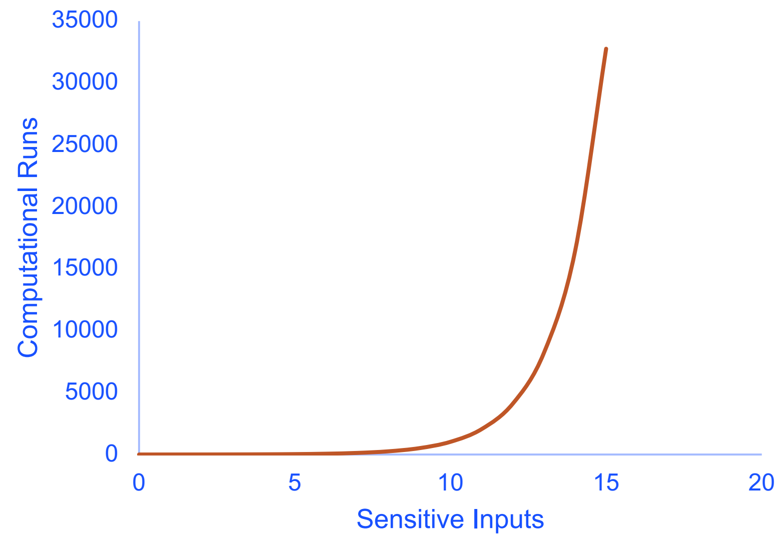
$$\%\ error\ in\ probability\ (P) = 200\sqrt{\frac{1-P}{NP}}$$

Ref. [3]

Propagation of aleatory and epistemic inputs can be computationally intractable.

How can sensitivity studies help?

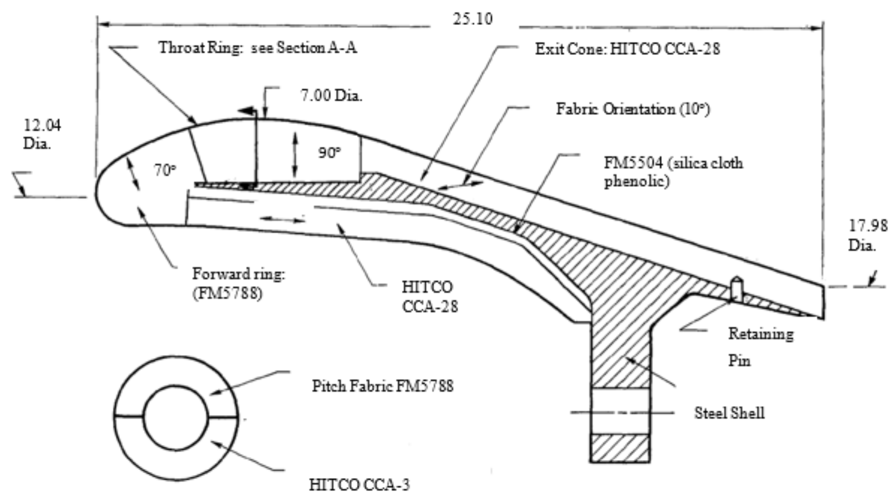
- Want surrogate model to represent computational model.
- Want surrogate model to be simpler and faster than computational.
- Only want inputs that matter in the computational model to be in the surrogate model.
  - Otherwise may have coefficients in surrogate model that are ~ 0 but waste computational time.
- Generating the surrogate model requires computational runs
  - number of computational runs depends on the number of inputs that may be sensitive and inputs that are sensitive.
  - $N_{sensitivity} = 1 + 2n_i$
  - $N_{surrogate} = 1 + 2^{n_f}$
  - $N =$ number of simulations
  - $n =$ number of sensitive inputs
  - $i, f =$ pre, post inputs in sensitivity analysis

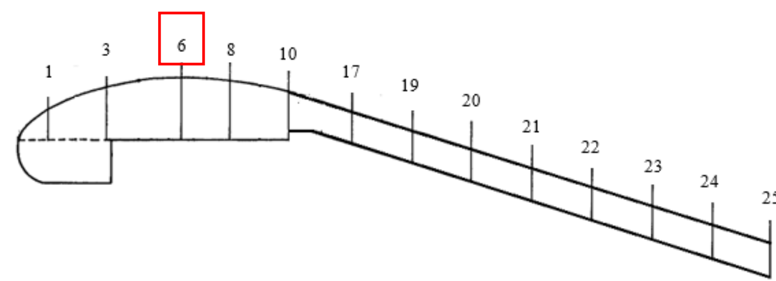


Number of inputs drives up computational cost of creating surrogate model.

Case Study

- 25-in rocket nozzle with 7-in throat[4]
- ~50 seconds of burn time
- ~650 psi average chamber pressure
- System response quantities of interest
  - Erosion depth at EOB
  - Char depth at EOB
- Modeling with ITRAC[5] and Chemics[6]
- Entire nozzle assumed to be MX4926 CCP.
- Apply surrogate model to throat (station 6).
- Geometry, material properties, boundary conditions, erosion and char data available in [4].
- CCP at throat about 2 inches thick.

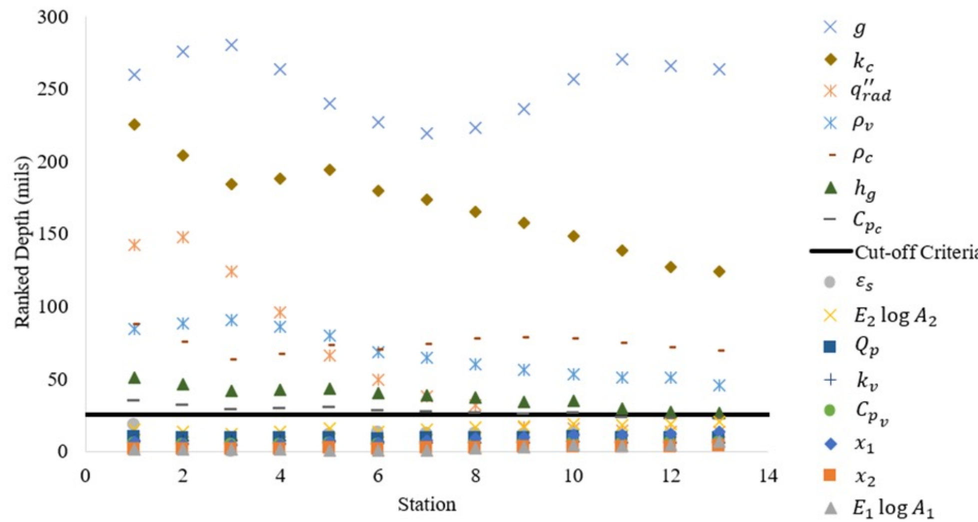




Throat of rocket nozzle used as case study.

Sensitivity of inputs in case study

- Looked at several inputs
- Local sensitivity analysis
- Ranked inputs based on erosion and char depth.
- Input had to be greater than 1% of erosion depth + 2% of char depth to be considered sensitive.
- Eight sensitive inputs:
  - enthalpy conductance
  - char thermal conductivity
    - Anisotropic behavior results in two inputs
  - Radiation heat flux
  - Virgin and char density
  - Pyrolysis gas enthalpy
  - Char specific heat.



$$Rank = \Delta E_{i-b} + 2\Delta C_{i-b} \geq 1\%E_t + 2\%C_t$$

Enthalpy conductance dominates erosion, char thermal conductivity dominates char.

Three techniques considered

- First technique uses ITRAC numerical derivatives from local sensitivity analysis.
- Second technique uses least square first order polynomial fit[7]
- Last technique uses poly-harmonic splines[8] to generate a surrogate model.
- Apply techniques to station 6 in nozzle geometry.
- Accuracy of surrogate model compared to ITRAC prediction of erosion and char depth at EOB.
- Computational efficiency based on computational effort to generate the model and propagate inputs through the model.
- Propagation based on 1000 aleatory runs and 500 epistemic runs.

Several techniques available in the literature to create surrogate models.

ITRAC numerical derivatives

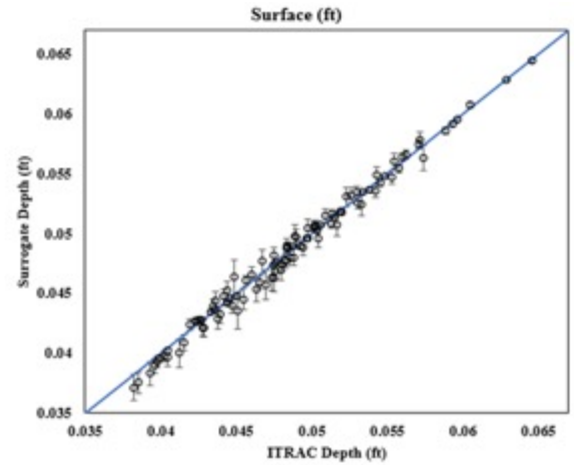
- Use the sensitive inputs
- Use a central difference numerical derivative at +/- 3 sigma.

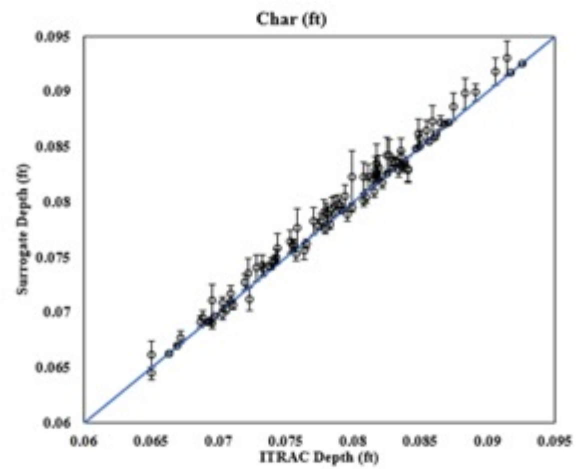
$$m_{ij} = \frac{\partial SRQ_j}{\partial x_i} \approx \frac{SRQ_j(x_i^0 + 3\Delta x_i) - SRQ_j(x_i^0 - 3\Delta x_i)}{6\Delta x_i}$$

- Y intercept is equal to the ITRAC SRQ output minus sum of numerical derivatives.

$$x_{0_j} = SRQ_j(\bar{x}) - \sum_{i=1}^{n} \frac{\partial SRQ_j}{\partial x_i}$$

- Relatively inexpensive to generate
- Number of simulations:
- $N_{sensitivity} = 1 + 2n_i$
- Results in a closed form first order polynomial
- Runs extremely fast
  - 500,000 surrogate simulations in a couple minutes on single processor

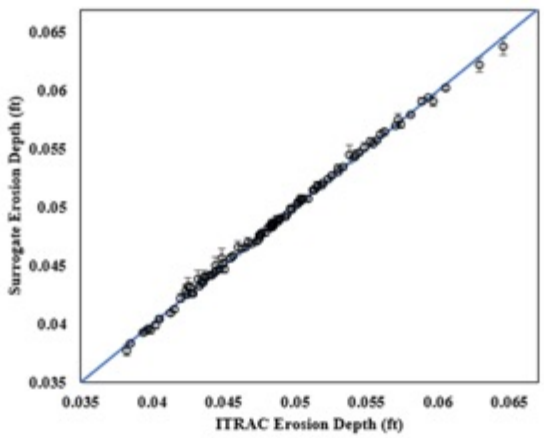


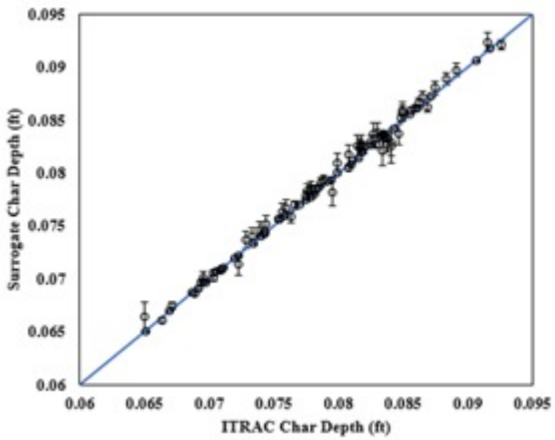


Surrogate model is within 15 mils of ITRAC for erosion and 30 mils for char.

First order least squares fit

- Requires the same sensitive runs as the ITRAC numerical derivatives.
- Build a surrogate model domain by running all sensitive inputs simultaneously at +/- 4 sigma.
- Run 100 LHC samples between +/-3 sigma in attempt to capture input interaction.
- $N_{surrogate2} = N_{sensitivity} + 101 + 2^{n_f}$
- More expensive than ITRAC numerical derivates to generate
- Just as fast to propagate uncertainties.
- Average error less than ITRAC numerical derivatives.

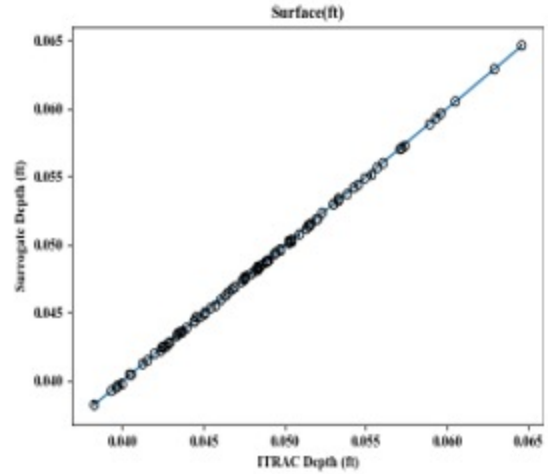


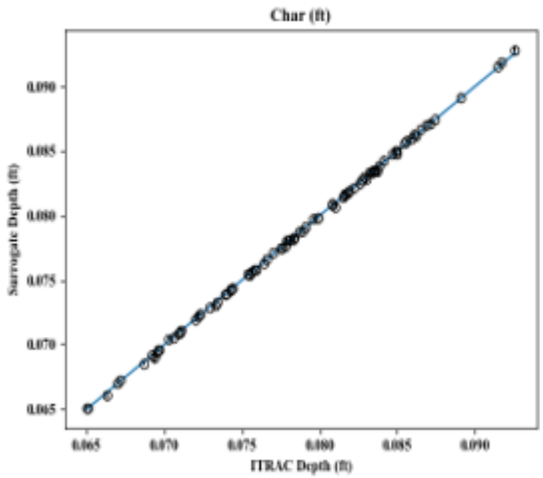


Surrogate model within 10 mils of ITRAC for erosion and 20 mils for char.

Poly-harmonic splines

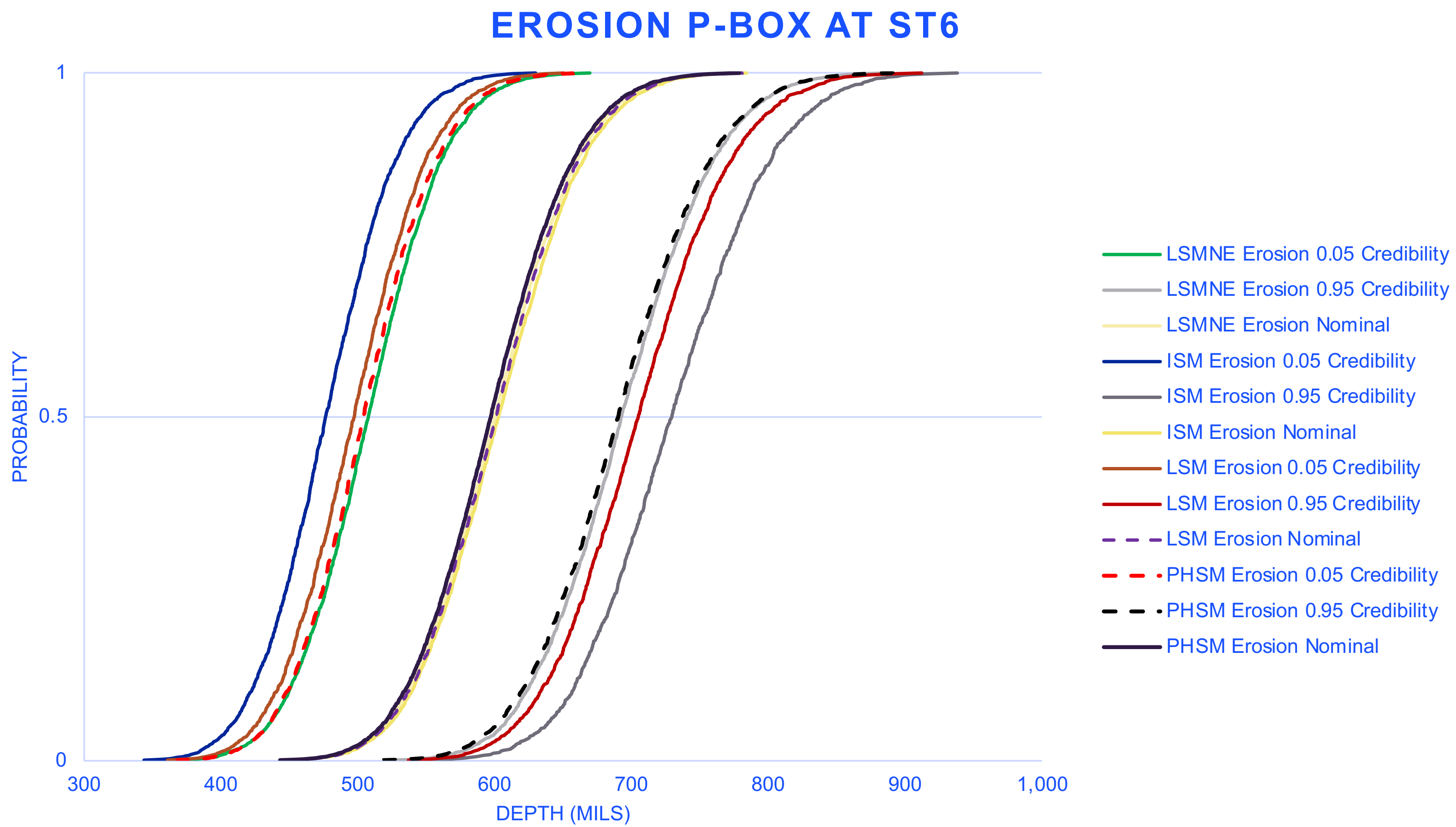
- Model is an interpolator at points it isn't fit at and has zero error where it is fit at.
- Requires same number of simulations as first order least squares.
- Can be given additional simulations for further fitting.
  - Sensitivity can be performed to find optimum number of fitting simulations.
  - More fitting required when erosion values get close to zero.
  - Model is not as stable outside of domain compared to linear model.
- Not a closed form model.
  - Can take 2-3 hours on six processor local machine compared to previous models taking less than a minute.
- Doesn't require any user interaction in the fitting or in error estimation.
- Additional fitting doesn't require user interaction.
- No error on erosion and minor error (a few mils) on char.
- Can reduce to zero error by giving more fittings points (say 200 more simulations)





Surrogate model equal to ITRAC for erosion and a few mils for char.

Comparison of surrogate models



Depending on other model form errors in the code itself, all these methods give reasonable results.

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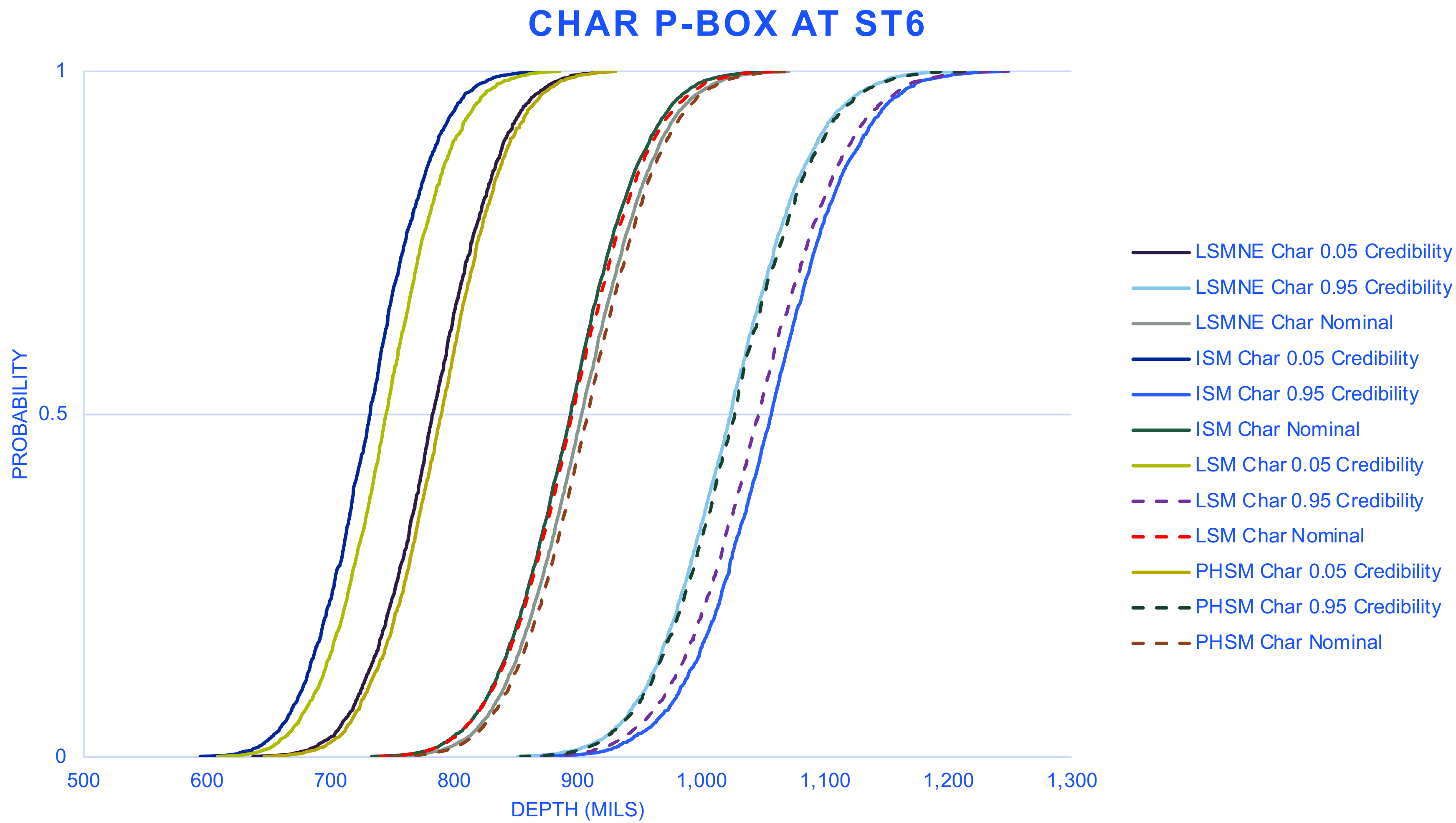

Depending on other model form errors in the code itself, all these methods give reasonable results.

Conclusions

- Surrogate models provide efficient and relatively accurate results compared to computational models.
- For propagation of input uncertainties, they are a necessity.
- Sensitivity analysis reduces the number of required simulations needed to generate surrogate models.
- Using ITRAC numerical derivatives from local sensitivity analysis provides an inexpensive approach with reasonable accuracy.
  - Accuracy can be improved by optimizing the y-intercept.
- Least squares polynomial fits provide improved accuracy but computational costs are an order of magnitude higher.
- Poly-harmonic splines provide an excellent fit with practically no error but are not as efficient as closed form models in propagating uncertainty and can have large error outside of domain.
- Recommendation for use depends on time available and desired accuracy.

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