CORRELATION OF THERMAL FLUID CRYOGENIC MODEL THROUGH IMPLEMENTATION WITH OPTIMIZATION SOFTWARE

Ellen K. Smith and Nathan F. Andrews
Southwest Research Institute

ABSTRACT

Predicting the effects of heat transfer with cryogenic fluids is an important but difficult problem for the space industry due to uncertainty in common heat transfer prediction correlations for boiling fluids. To mitigate some of this uncertainty, predictive thermal fluid models can be anchored to experimental data prior to conducting exploratory studies using the model. Doing so enables rapid engineering in the early stages of component- and system-level design trades. This paper presents a technique employing CENTAUR™ (Collection of Engineering Tools for Analyzing Uncertainty and Reliability), an optimization software, to calibrate a simple thermal fluid model for simulating the chilling of a cryogenic propellant line. Experimental data available in the open literature is used to calibrate the predictive model.

INTRODUCTION

Predicting the effects of heat transfer with cryogenic fluids is an important step in the design of many cryogenic space system, but it is a difficult problem to accurately model, particularly in the early stages of a system's design. The challenge is largely due to uncertainty inherent in the commonly used empirical boiling correlations, which leads to carrying excess margin in vehicle design. To mitigate some of the effects of this uncertainty, initial models can be anchored to experimental data before exploratory studies are conducted using the model. The process of anchoring the model can be challenging and tedious and does not always result in an acceptable data match. This paper presents a technique employing an optimization software to automate and run model dispersions, query the resulting predictions for comparison against available experimental data, and then tune model parameters to improve the accuracy of the model. The optimized parameter set can then be used for the design of a new system.

MODEL IMPLEMENTATION

The following study demonstrates this approach for a thermal fluid model of a cryogenic line chilling operation, built to replicate the experimental setup tested in [1]. The model of the system was developed in ANSYS Thermal Desktop version 6.1, patch 40 (with Sinda/Fluint version 6.1, patch 41 and Intel Visual Fortran 6.1) [1]. Thermal Desktop is a graphical user interface to the Sinda/Fluint solver implemented in an AutoCAD framework and is used for advanced pre- and post-processing capabilities such as automating complicated geometry calculations. Sinda/Fluint is a lumped parameter and finite difference solver for 3D thermal and 1D fluid analysis with aerospace heritage dating back to the 1960's.

The model setup in Thermal Desktop is shown in Figures 1 and 2. Liquid nitrogen enters the test section from a constant temperature source at a constant flow rate enforced by the mass flow set element. The experiment tested 3 flow rates, but this study only explores a single flow rate corresponding with a Reynolds number of 5992. The test section is modeled using Thermal Desktop pipe elements with junction lumps and diffusion wall nodes. Short paths with negligible losses are used to connect the pipe elements and the source and sink plenums. The test section is a vertical stainless-steel pipe with a 1.168 cm inner diameter, installed almost entirely in a vacuum chamber. There are two short sections on either side of the vacuum chamber that are exposed to the atmosphere but are insulated with aerogel. These sections are modeled separately to account for the differences in insulation and external heat transfer. The heat transfer ties to the exterior of the aerogel insulation on the exposed section is modeled as natural convection to an isothermal vertical cylinder. The heat transfer ties to the exterior of the test section inside the vacuum chamber is also modeled as natural convection to an isothermal vertical cylinder, but with an air pressure of 1.3 Pa rather than atmospheric pressure. The heat transfer from the liquid to the internal walls of the test section is modeled using correlations for fluid flowing within a pipe.

Two key items must be noted regarding the experimental report and the modeling approach. First, the pipe inlet (source) liquid temperature and the environment temperature were not explicitly provided in the experimental documentation. These values must be assumed in the model and represent a key uncertainty source for the purposes of this demonstration. Second, the thermal fluid model was initially built using the default heat transfer correlations available in the software. This represents the second major source of uncertainty scrutinized in this study. Also note that experimental pipe wall temperature data is presented from only two thermocouple locations, shown in Figure 3(denoted in this study as upstream and downstream locations).
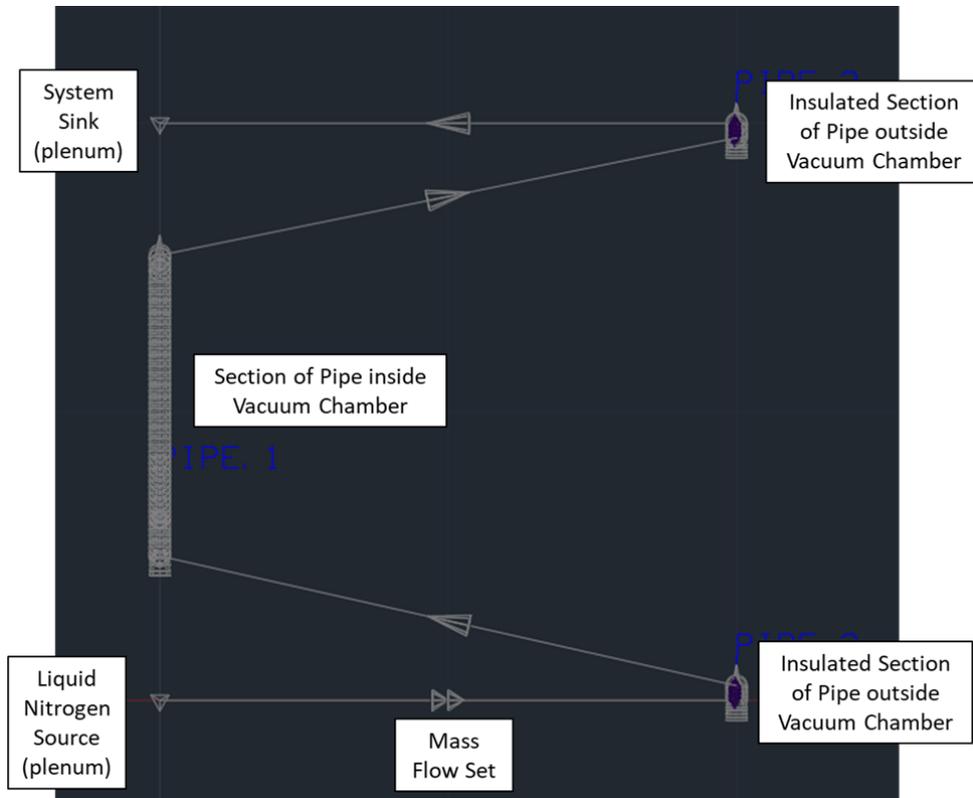
Figure 1. Schematic of how flow of the chilldown experiment from [1] was modeled in Thermal Desktop.
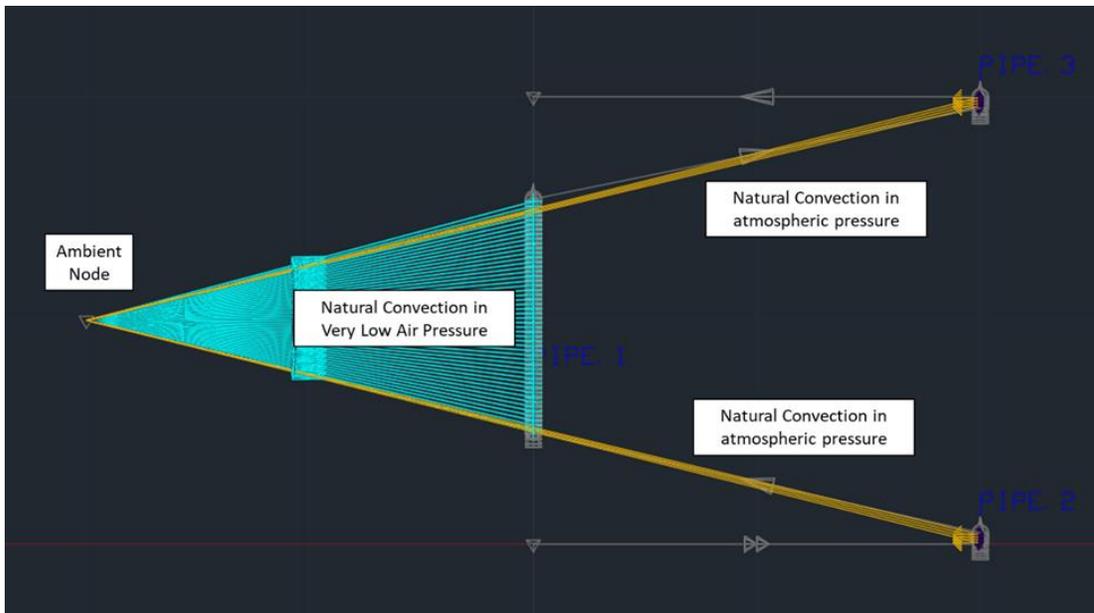
Figure 2. Schematic of how external heat transfer to the test section during the chilldown experiment from [1] was modeled in Thermal Desktop.
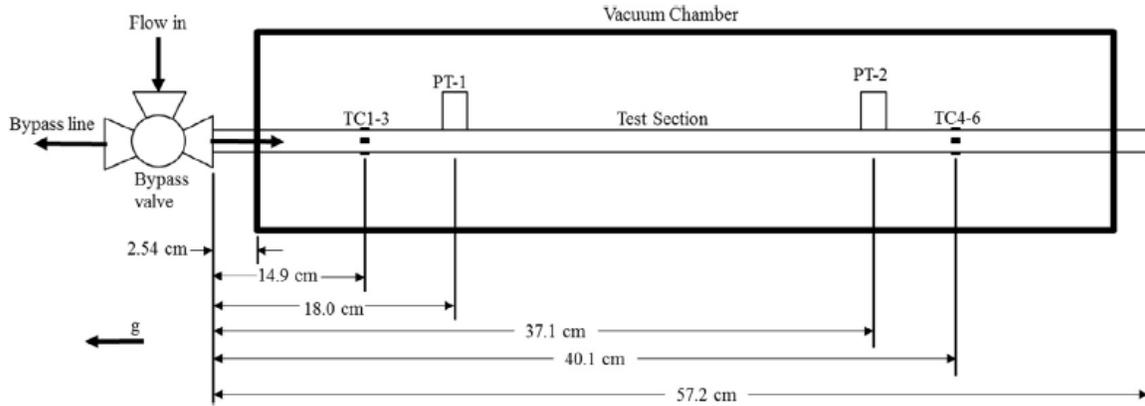
Figure 3. Schematic of experimental test setup with specifics of on temperature sensor placement [1].

Rather than performing a manual calibration, an optimization software, CENTAUR, was employed for a quick and systematic approach. CENTAUR is the engine behind another general-purpose probabilistic analysis software, NESSUS [3], but can also be directly utilized as a standalone package. This direct interfacing allows for the customization of uncertainty quantification (UQ), surrogate modeling, model calibration, and optimization solution approaches via Python or MATLAB [3]. For design of experiment (DOE) generation, many sampling methods are available including Monte Carlo, Latin-Hypercube, and Sobol sampling. Response surface methods include high-order polynomial regression with interactions and Gaussian process (GP) models, which are appropriate for fitting complex, nonlinear functions with limited computer simulations. Both global and gradient-based optimization methods are supported, as well as Bayesian calibration methods for reflecting residual uncertainty after model fitting.

For this study, the CENTAUR software library was used, through a Python interface. The script was written to invoke Latin-Hypercube sampling to generate the DOE and response surface training data, train a GP response surface to represent the model's root-mean-square (RMS) error against experimental data, and optimize the thermal fluid model to find the combination of input parameters which minimize an objective function. Using Thermal Desktop's OpenTD interface, Python calls Thermal Desktop, updates the model parameters and runs through the DOE dispersion cases automatically. Once the model cases and training data are complete, the script pulls the pertinent results, generates the GP response surface model and uses a global optimizer on the GP model to return the parameter values that minimize the objective function.

Three parameters were chosen for tuning the model to match experimental data. These parameters were selected to target the two uncertainties highlighted previously, namely the source liquid temperature, ambient temperature, and pipe internal heat transfer multiplier. The pipe internal heat transfer multiplier modifies Thermal Desktop's default heat transfer coefficient from the liquid to the internal walls of the test section. Expected ranges for these variables were: liquid temperature from 70 to 100 K, ambient temperature from 280 to 320 K, and pipe internal heat transfer multiplier from 0 to 2. Running 300 dispersion cases was ultimately chosen because of recommendations for the DIRECT (Dividing RECTangles) optimizer [1]. In this demonstration, the upstream pipe wall temperature RMS error from the experimental results was used as the objective function. The

temperature of the downstream sensor was used as for model verification independent of the training.

MODEL CALIBRATION RESULTS

Comparison of the uncalibrated model and experimental results of the upstream wall temperature sensor are shown in Figure 4. The comparison was performed on data at the upstream thermocouple location and at the lowest tested flow rate, a Reynolds number of 5992. The uncalibrated model assumes an ambient temperature of 300 K, a liquid temperature of 80 K, and a pipe internal heat transfer multiplier of 1, which results in a poor prediction for the wall chill down.

The calibrated model is a better match and predicts wall temperature within 6% RMS error. This is also shown in Figure 4. The optimal parameters for liquid temperature and ambient temperature are only slightly altered from the assumptions of the original model, to a liquid temperature of 77.7 K and an ambient temperature of 280.0 K. However, the optimal pipe internal heat transfer multiplier is significantly lower than the default of 1, at value of 0.354. This indicates that the default Thermal Desktop heat transfer correlation is a significant contributor to the overprediction of the heat transfer from the cryogenic liquid to the internal walls of the pipe.
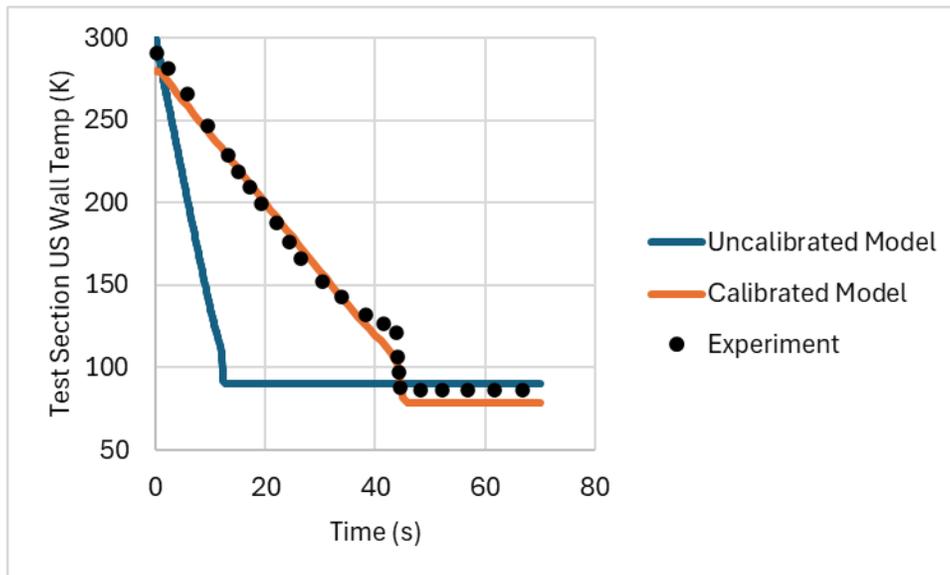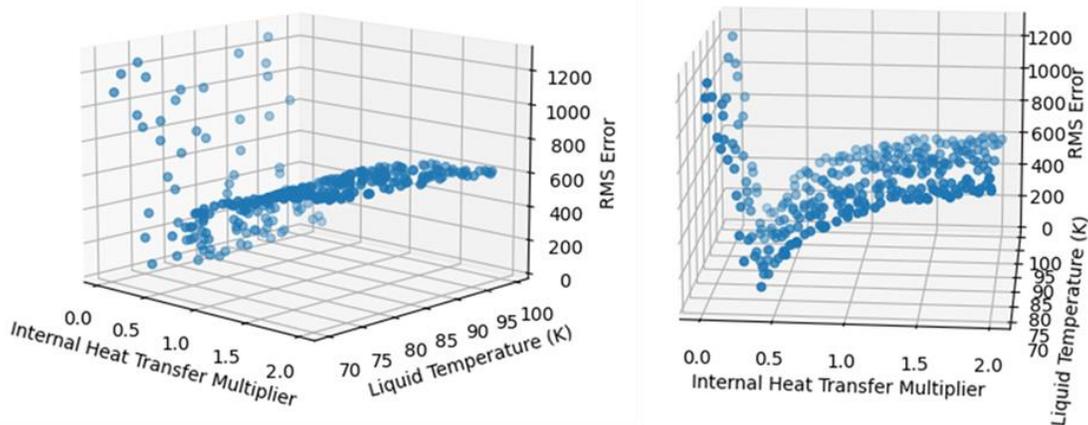

Figure 4. Comparison of outer test section wall temperature at the upstream temperature station at a steady state Reynolds number of 5,992 between the uncalibrated and calibrated models and the experimental data.

Visualizing DOE parameters spaces and response surfaces with three degrees of freedom is awkward, so simplified results were generated using two variables while holding the third constant. These are shown in Figures 5 and 6. Both figures show two views of the same plot for better visual clarity. Figure 5 presents the design space and the predicted RMS error from the experimental upstream wall temperature while varying pipe internal heat transfer multiplier and ambient temperature but holding liquid temperature constant. Figure 6 presents the RMS error while

varying pipe internal heat transfer multiplier and liquid temperature but holding ambient temperature constant. The figures show that the model is very sensitive to internal heat transfer multiplier but minimally sensitive to ambient or liquid temperature. A clear minimum valley can be observed in each of the three-dimensional domains.
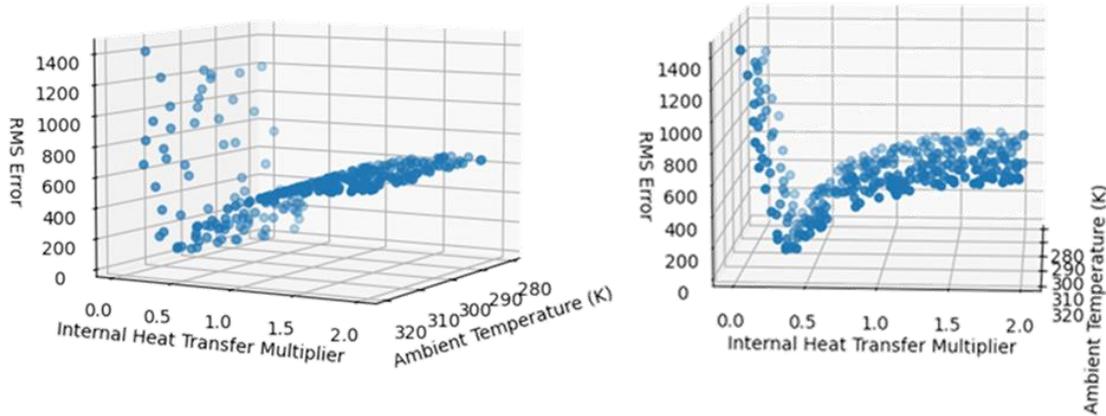

Figure 5. Figures showing the RMS response surface from DOE while holding liquid temperature constant at 86 K.

Figure 6. Figures showing the RMS response surface from DOE while holding ambient temperature constant at 291 K.

Using the calibrated model, a comparison of downstream outer test section wall temperature was also made, as shown in Figure 7. Unfortunately, the match to the downstream wall temperature is lower quality than the trained upstream section. The model predicts very similar upstream and downstream wall temperatures despite the difference in temperature along the length of the pipe wall seen in the experimental data. This is likely because the external heat transfer of the vacuum chamber should have been included in the set of calibration parameters. This disparity emphasizes the importance of understanding the model sensitivity to parameters and weighing confidence in each model parameter. It also emphasizes the significance of having multiple model validation

points. Still, for the purposes of this study, the demonstration is adequate to show the engineering process for improving the model and exploring sensitivity of the model prediction.
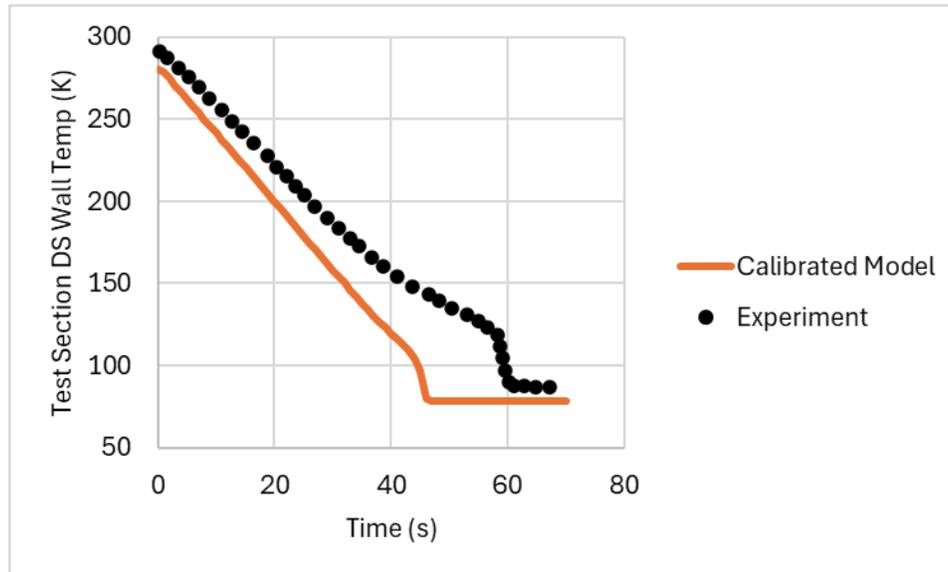
Figure 7. Comparison of outer test section wall temperature at the downstream temperature station at a steady state Reynolds number of 5,992 between the calibrated model and the experimental data.

CONCLUSION

Although the model in this study is simplistic and did not examine the appropriate parameter set to also match downstream test section wall temperature, the process described can be applied to much more complicated models and situations. Our experience has shown that following this process, with additional model tuning, parameter exploration, and data comparison can greatly improve the tuning results and predictive capability of early engineering thermal fluid models for engineering design. The process provides a time efficient method for tuning models to experimental data so that additional design studies and off-design cases can be considered.

REFERENCES

[1] S. R. Darr, N. G. Glikin, J. W. Hartwig, A. K. Majumdar, A. C. Leclair and J. N. Chung, "An experimental study on terrestrial cryogenic transfer line chilldown I. Effect of mass flux, equilibrium quality, and inlet subcooling," *International Journal of Heat and Mass Transfer,* no. 103, 2016.

[2] "ANSYS Thermal Desktop," [Online]. Available: https://www.ansys.com/products/fluids/ansys-thermal-desktop.

[3] "NESSUS," Southwest Research Institute, [Online]. Available: https://www.swri.org/centaur. [Accessed 2024].

[4] "Centaur," Southwest Research Institute, [Online]. Available: https://www.swri.org/centaur. [Accessed 2024].

[5] D. R. Jones and J. R. R. A. Martins, "The DIRECT algorithm: 25 years later," *Journal of Global Optimization,* 2020.