

Smoothing the Path to Simulation-Led Device Design

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Abstract: Using modeling software such as COMSOL Multiphysics during the early design phase, an approach called “simulation-led design”, allows ideas to be both inspired and validated by the use of simulations. Later, using simulations after the product is designed can shorten the prototype-testing portion of the development process and reduce its cost.

This paper provides specifics on the nature of the design innovation process, showing a sample model of a pipeline gasket using the Non-isothermal Laminar Fluid Flow interface in the CFD module, some of the variations possible, and plots that were useful for communicating the design performance data.

Using the modeling tools and graphics options provided by COMSOL Multiphysics was shown to be effective for the development of design ideas and for communicating these designs.

Keywords: design, laminar, fluid, flow, solder, simulation-led, phase transition, CFD.

1. Introduction

New product design is challenging in today’s competitive market environment. It is necessary to use effective techniques that can shorten the time from product inspiration to commercialization. An approach called “simulation-led design”, allows ideas to be both inspired and validated by the use of simulations, in addition to the benefits of using simulations after the product is designed to shorten the prototype-testing portion of the development process and reduce its cost.

Pryor Knowledge Systems has used COMSOL Multiphysics models as part of effective product design consultations with our clients. This paper will describe an application in which we used this simulation-led design technique to explore several approaches that would meet our client’s requirements.

This model was built in order to evaluate metallic materials, to be used to repair breaches in the pipe or as a gasket between piping sections, that would retain their integrity within the expected environmental heat range during the repair process. Known quantities were: the dimensions of the pipe, the velocity and temperature of heated material flowing through the pipe during repair, and the temperature of the environment surrounding the pipe.

The model will use a rectangular section of the toroidal gasket material, which is symmetric around the vertical axis. See Figure 1.

2. Methods

This example illustrates methods for setting up a model that allow easy changes to a design to facilitate research into the variables within constraints. This model demonstrates the following techniques: 1) the use of global parameters, 2) the use of model-level variable expressions, 3) the use of probes, and 4) the use of plots to ensure that the design is meeting specifications.

This model uses the value of the heat capacity when the material undergoes a phase change to determine whether the material and/or geometry is a candidate for a practical solution to the problem.

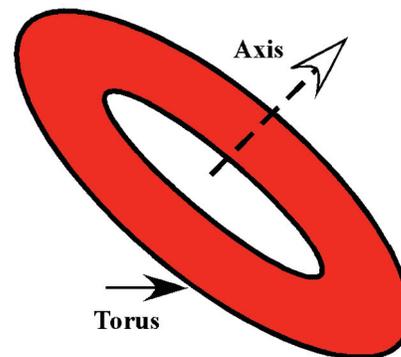


Figure 1. Toroidal Disk Modeled [2].

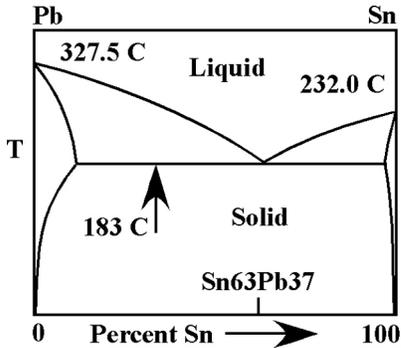


Figure 2. SnPb Phase Diagram [2].

It uses similar phase-change approaches illustrated by COMSOL [1] and Pryor Knowledge Systems [2] in previous models, with an emphasis in this paper on building into the model the flexibility for the exploration of various candidate materials.

2. Governing Equations

The materials considered in this model are eutectic alloys, which will be processed in the 380K – 480K temperature range. At those temperatures, the material properties of interest in this model, the heat capacity and thermal conductivity, are dominated by electron energy transport. Experimentally, in this temperature range for these materials, the heat capacity can be expressed as:

$$1. C = \gamma T + AT^3$$

where γ and A are material-specific constants [3] and the phonon contribution (AT^3) is very small compared to the electron contribution.

The thermal conductivity (K) is related to the heat capacity per unit volume as:

$$2. K = \frac{1}{3}Cvl$$

where C is the heat capacity per unit volume, v is the electron velocity and l is the mean free path [4].

3. Use of COMSOL Multiphysics

3.1 Creating the Model

We created a new model using the COMSOL Multiphysics Model Builder wizard. This will be a 2D Axisymmetric model, using the Fluid Flow > Non-Isothermal Flow – Laminar Flow (nif) physics option, and a study type of Stationary.

3.2 Using Global Definitions

We added a Parameters list to the Global Definitions header. This section will define the constants that will be used in the model, as shown in Table 1 in the Appendix. The table shows the names assigned to the parameters, their values, and the description of their use in the model. Setting up as many data items as constants as possible allows the model builder to change the model parameters in one place, and then refer to them by name in the model settings pages, rather than entering constant values in fields scattered throughout the model. This approach facilitates innovative design by setting up a model in which it is easier to vary the conditions when running multiple design scenarios.

3.3 Using Model Variables

Next, under Model > Definitions, we added a Variables list that defines the expressions for terms that will be used in the model. See Table 2 in the Appendix for the list of the expression names, values and descriptions. These expressions capture the physics related to handling the properties of a material. We set the geometry entry level to All Domains.

3.4 Setting Up the Geometry

The geometry is a simple rectangle, offset from zero, representing a cross-section of the toroidal gasket material. The settings all use the global parameters to retain flexibility in the design.

We also changed the Axis settings in the default View to reflect the separate r and z (x and y) scaling needed. See Figure 3.

3.5 Material Definition

We defined our gasket material, using the parameters and variable expressions, and changed

the default name to identify which material was being modeled in each instance.

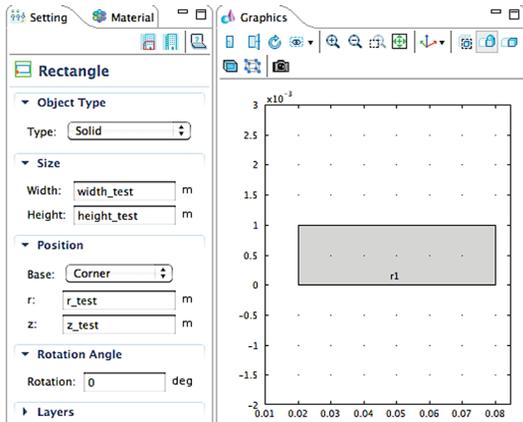


Figure 3. The geometry settings illustrate the use of global parameters.

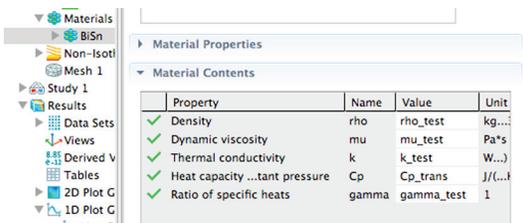


Figure 4. The material properties use global parameters and model variables.

3.6 Non-isothermal Flow Physics Settings

As a result of the particular volume-force term in the momentum equation for this mode, for the consistent stabilization heat and flow equations, we used only streamline diffusion, not crosswind diffusion, to improve convergence. Under advanced settings, we removed the pseudo time stepping, because for convection flux we needed the smaller scale associated with phase transition. Under discretization, we chose the P2 +P1 option because the quadratic form better represents the behavior of the velocity and temperature fields.

The initial values were set using the parameter u_cast and zero for the r and z elements of the velocity field vector, and the temperature T was set to the parameter T_in , to preserve the flexibility of the model. We also ensured that the fluid properties would take their values from the material.

The volume force settings for Laminar Flow were defined using the parameters $-Sr$ and $-Sz$. The Laminar Flow inlet was set to the boundary associated with the interior surface of the gasket. The velocity and inlet size entries were set using the global parameter names.

The Laminar Flow outlet was set to the boundary associated with the exterior surface of the gasket. The boundary condition, pressure, was selected and set to zero.

The Laminar Flow boundary condition, symmetry, was assigned to the other two boundaries, which represent the edges of the section of gasket material.

The model also required a Heat Transfer temperature boundary condition for both the interior and exterior surfaces of the gasket. These were set to the global parameters T_in and T_out respectively.

The Thermal Insulation condition was applied to both of the other boundaries.

3.7 Setting Up a Probe

We used a probe to provide a snapshot view of the heat capacity value at one point in the center of the material. Since we planned to run a parametric solver, the results would be a data set of the heat capacity values at that point. The results were plotted as the solution was run. See Figure 5 for the setup in the builder tree, the settings for the point probe value and the resulting plot.

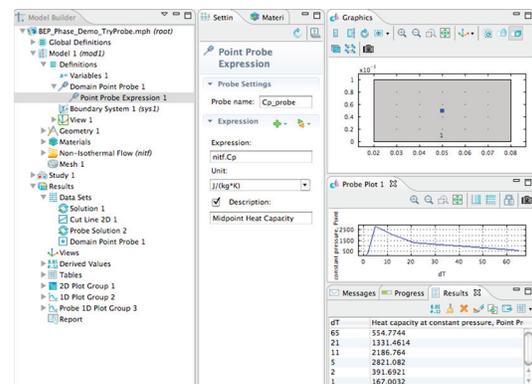


Figure 5. Setup and results for a point probe.

3.8 Meshing

We set the meshing to be physics-controlled and set the element size to extra coarse, giving us approximately 2500 elements, which was sufficient for the simple geometry to show us the temperature change across the gasket section.

3.9 Setting Up the Parametric Solver

We modified the default settings of the stationary solver by adding a continuation extension, using the parameter, dT , which represented the half-width of the temperature transition zone, as the continuation value. A list of values: 65; 21; 11; 5; 2 and 1, were used to specify a variety of sizes of the region between the liquid and solid phases, making the transition point easier to identify.

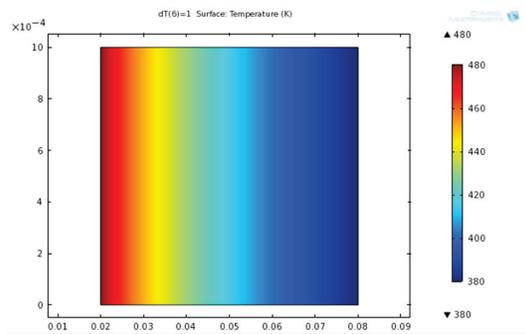


Figure 6. The surface plot shows the range of temperatures across the heated gasket material.

4. Results

The transition temperature for this BiSn material is 411.15K, which is reached when $r=0.0549$ m. See Figure 6.

An additional 1D plot of the heat capacity of the material for the set of dT values along a cut line at $z=0.001$ m, confirms the phase transition point. See Figure 7.

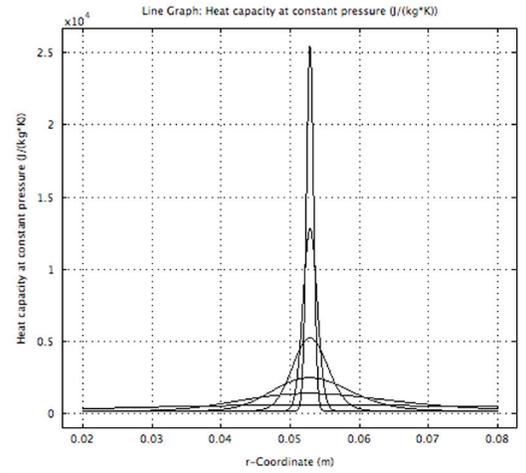


Figure 7. Heat capacity across the heated gasket material.

5. Conclusions

COMSOL Multiphysics provides several tools that support innovative design efforts by allowing the modeler to build flexibility into exploratory models. The ability to use global and local parameters, local variables, probes and plots enhanced our project as we evaluated various materials for their suitability and communicated those results to our client.

6. References

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2. Pryor, R. W., Modeling Materials through a Phase Change: Using COMSOL Multiphysics and Applying Physics First Principles Techniques, *Proceedings of the COMSOL Conference*, 1-7. COMSOL, Boston (2007).
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4. C. Kittel, Eutectics, *Introduction to Solid State Physics*, **6th Edition**, 150 (1986).

7. Appendix

Table 1: Global parameters.

Name	Value	Description
T0	300[K]	Initial temperature

Name	Value	Description
T_in	480[K]	Temperature in
T_out	380[K]	Temperature out
dT	0.5[K]	Temp half width of transition zone
dH	44.8[J/g]	Change in enthalpy
u_cast	1e-5[m/s]	Velocity of the cast item
T_trans	411.15[K]	Transition temp of tested solder
Cp_test	0.167[J/(g*K)]	Heat Capacity of tested solder
rho_test	8.56[g/cm ³]	Density of tested solder
mu_test	0.01[Pa*s]	Dynamic viscosity of tested solder
k_test	0.19[W/(cm*K)]	Thermal conductivity of tested solder
gamma_test	1	Ratio of specific heats
width_test	0.06	Width of test piece
height_test	0.001	Height of test piece
r_test	0.02	r offset from corner of test piece
z_test	0	z offset from corner of test piece
L_entr	1e-3[m]	Inlet entry length

Table 2: Model variables.

Name	Expression	Description
D	$\exp(-(T - T_{trans})^2 / (dT^2)) / \sqrt{\pi * dT^2}$	Temp dependence, latent heat
B	$(T - T_{trans} + dT) / (2 * dT) * ((T$	Fraction of liquid phase

	$\leq (T_{trans} + dT) * (T) = (T_{trans} - dT)) + (T > (T_{trans} + dT))$	
Sr	$(1 - B)^2 / (B^3 + 1e-3) * 1e5 [kg / (m^3 * s)] * (u_{cast})$	Volume force density, r-component
Sz	$(1 - B)^2 / (B^3 + 1e-3) * 1e5 [kg / (m^3 * s)] * w$	Volume force density, z-component
H	$f_{lc} 2hs (T [1/K] - T_{trans} [1/K], dT [1/K])$	Enthalpy
Cp_trans	$Cp_{test} + (D * dH)$	Heat capacity modified by latent heat released