Linear Convection and Conduction in Cylinders of Water Exposed to Periodic Thermal Stimuli

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Introduction

Primary reference standards for determining absorbed dose to water in radiotherapy beams used at cancer clinics and hospitals ultimately must make reference to the temperature change in water produced by ionizing radiation. The most direct experimental technique for this purpose is water calorimetry, in which a volume of ultrapure water is exposed to a beam, and the rise in temperature is measured via thermistor probes. Since the dose distributions delivered by such beams are nonuniform, temperature signals generally exhibit distortions due to heat conduction and convection, making it necessary for the determination of appropriate correction factors.

In virtually all such metrology applications throughout the world, heat-transfer distortions are minimized by restricting exposure times and using long equilibration intervals to allow for the decay of temperature gradients. Finite-element analysis then is used to model the transient response of the calorimeter vessel to conduction and convection in order to obtain the desired correction factors. With the help of COMSOL Multiphysics, we have been able to develop an alternative approach to the problem that characterizes the thermal frequency response of the calorimeter vessel to periodic irradiation, thereby allowing us to dispense with the equilibration intervals and greatly improve the effective experimental duty cycle.

As part of this work, we have been investigating the feasibility of using a high-precision temperature bath to study the thermal frequency response of the water calorimeter vessel independently of the radiation beam. The bath, which enables us to control both the amplitude and timing of thermal stimuli, is suitable for measurements of the system transfer function which can be compared to output of finite-element simulations. A major benefit of the bath experiments is the degree to which we can control the amount of convection in the cell by independently varying the mean temperature and the amplitude of temperature oscillations, thus enabling us to isolate its effects separately from those of conduction in ways that would not be possible in the target radiation environment. By successfully modeling the heat transport over the range of conditions obtainable with the bath, we hope to arrive at a robust system transfer function that would enable us to correct our measurements for heat transfer for arbitrary timing characteristics of the radiation field.

Use of COMSOL Multiphysics

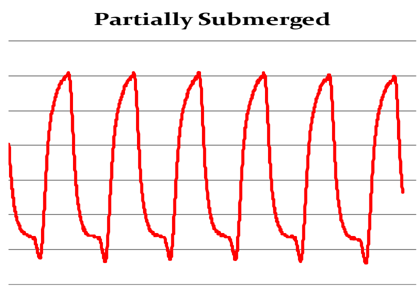
The calorimeter vessel is a hollow cylinder constructed out of ~0.4 mm glass with a diameter of ~2 cm and a length of ~12 cm. The interior contains ultrahigh purity water and the entire vessel is immersed in a water bath whose temperature we control via computer. We have alternately used time-dependent solvers in both the Heat Transfer Module and the basic package (viz. conduction/convection and incompressible Navier Stokes equation systems) to model heat transfer within the vessel and between the vessel and external environment. In the simpler implementations, the latter is modeled with a temperature or flux boundary condition that is periodic in time. Among the questions we have addressed or plan to address are the following:

- What imperfections in the shape of the vessel are ignorable?
- How far may temperatures deviate from 4 ^{o}C before convection phenomena are observable?
- To what extent are attenuation and phase shift in the transfer function sufficient to characterize convection in the calorimeter (i.e. under what conditions do nonlinearities become significant)?
- Can simulation results help us to identify an analytical expression with adjustable parameters that could be determined via chi-square minimization (involving experimental data)?
- How to estimate systematic errors in our data analysis that arise from our simulations?

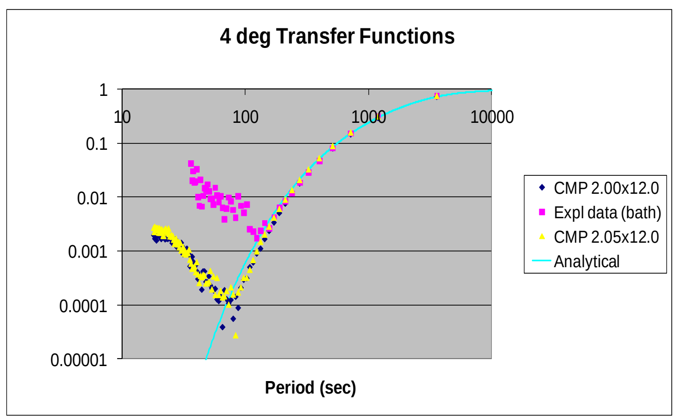
Expected Results

The seeming simplicity of our physical system – a cylinder containing water subject to small, periodic temperature perturbations – is somewhat beguiling, exhibiting phenomena that are suggestive of analogies to simple a.c. electrical circuits yet differing enough quantitatively from them that multiphysics models are essential to obtaining accurate estimates of our desired quantity. COMSOL Multiphysics has been quite helpful in both qualitative and quantitative aspects of this problem, enabling us to understand the origin of various phenomena we observe in the cell and helping us to estimate the associated correction factors. We provide just two examples.

The temperature overshoot in the first figure below illustrates one of the phenomenological surprises that we were able to understand and quantify using multiphysics modeling. The waveform in the figure represents thermistor response, obtained along the vessel axis, to a square-wave temperature stimulus applied to the outside of the vessel. The waveform exhibits the low-pass type distortions due to heat conduction that one would expect from the layer of water separating the sensor from the wall of the vessel. However, heat conduction would not explain either the difference in rise/fall times or the overshoot just prior to the transition edges. Closer inspection of the experimental setup suggested a possible cause – partial submersion of the vessel producing a static temperature gradient along the cell that effectively amplified the consequences of convection at the point of measurement – and, using COMSOL Multiphysics, we were able to reproduce the artifact in our data very well.



We have also made good progress with regard to quantifying these effects sufficiently for purposes of parametrizing transfer functions and obtaining correction factors for heat transport. The figure below compares experimental measurements with both COMSOL Multiphysics output and an analytical solution to the heat conduction problem for one of our calorimeter vessels in the bath at 4 ^{o}C, where the thermal expansion coefficient of water is near zero (and convection is effectively shut down). The agreement among all curves is excellent at longer shutter periods and continues to be good down to shutter periods of about 200 seconds, at which point random uncertainty in the experimental data begins to dominate (shown by the sudden upward direction of the magenta markers). The agreement among all curves over the range of experimental precision is nevertheless excellent and suggests that the prospects for obtaining a physically-motivated transfer function and, hence, the desired correction factors for our calorimeter are quite good.



Conclusion

Multiphysics simulations have proven to be exceedingly useful in our development of an alternative approach to water calorimetry that eliminates experimental down time present-day systems require for reestablishing thermal equilibrium throughout the course of a run. With COMSOL Multiphysics, we have been able to address numerous questions about the physics of convection and conduction in water calorimeters that have hitherto not been investigated quantitatively. As radiotherapy for cancer makes greater use of modulated beams, adaptations of our approach may prove to be quite valuable in the development of new generations of primary reference standards.