3D Simulation of Air-Glass Heat Exchange in a Set of Vials.

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Model Set-Up: We consider the heating of a set of vials in a current of hot air in the laminar regime. Our main purpose is to determine the internal surface temperature $T(\mathbf{x},t)$ of the glass vials as a function of space and time.

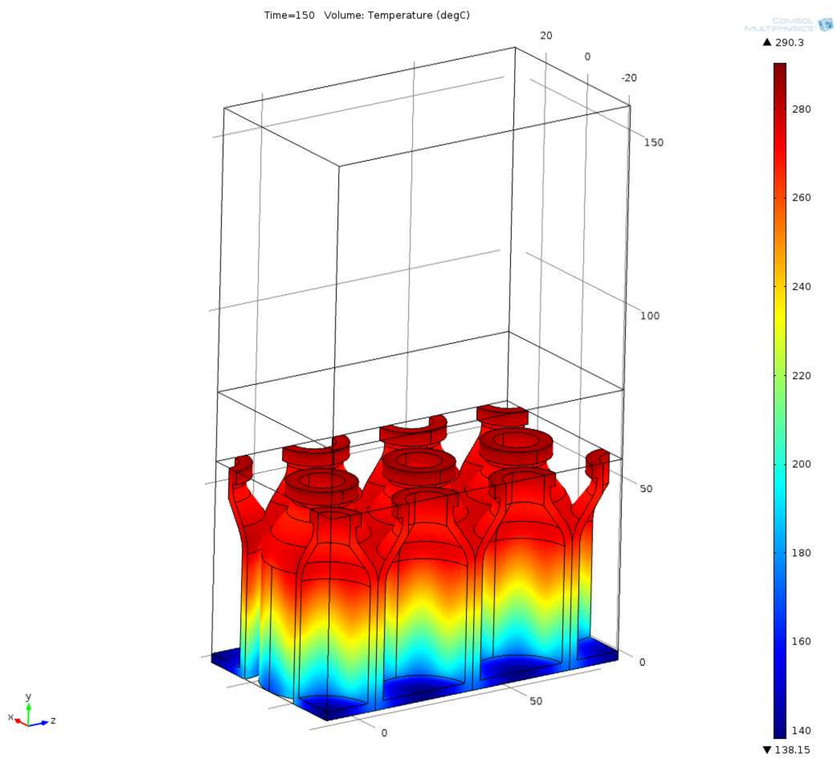

Figure 1. The Model.

Governing Equations and Computational Methods: To look through FEA numerical solutions we used a *Time Dependent Study* based on the Conservation Equations for Non Isothermal Fluids and the Heat Equation (with appropriate boundary conditions):

$$\frac{\partial \rho}{\partial t} + \nabla_x \rho \cdot \mathbf{u} + \rho(\nabla \cdot \mathbf{u}) = 0.$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \frac{1}{\rho} \nabla \cdot \left[-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right].$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{\rho c_p} \nabla \cdot k \nabla T.$$

$$\frac{\partial T}{\partial t} = \frac{1}{\sigma \xi_p} \nabla \cdot \kappa \nabla T.$$

Where ρ is the air density, $\mathbf{u}$ is the air velocity, c_p and k are respectively the heat capacity and thermal conductivity of air. Instead in the last equation σ, ξ_p and κ are respectively the density, the heat capacity and the thermal conductivity of the vials material (glass).
For the solution with COMSOL Multiphysics we have used a Direct Solver; where possible we have chosen a Fully Coupled solver, and when the degrees of freedom were more than one million we have used a Segregated solver.

The simulation allows us to know the function of temperature $T(\mathbf{x},t)$. With a *Global Equation* node we defined a first order ODE and we estimate the following function of fundamental importance in the sterilization and depyrogenation of vials (T_0 and z are constants):

$$F_H = \int_0^t 10^{\frac{T(\tau)-T_0}{z}} d\tau.$$

Results: The comparison between the simulation results and experimental data indicate that in presence of sufficiently dense mesh, the absolute error of the function of temperature is particularly low (definitively less than 5 ° C). In addition also the estimation of F_H, in the case simulated, appears cautionary and therefore acceptable (see Figure 4).

Figure 2 shows the trend of the error between the internal temperature in two different simulated samples and the internal temperatures in a vial experimentally measured.

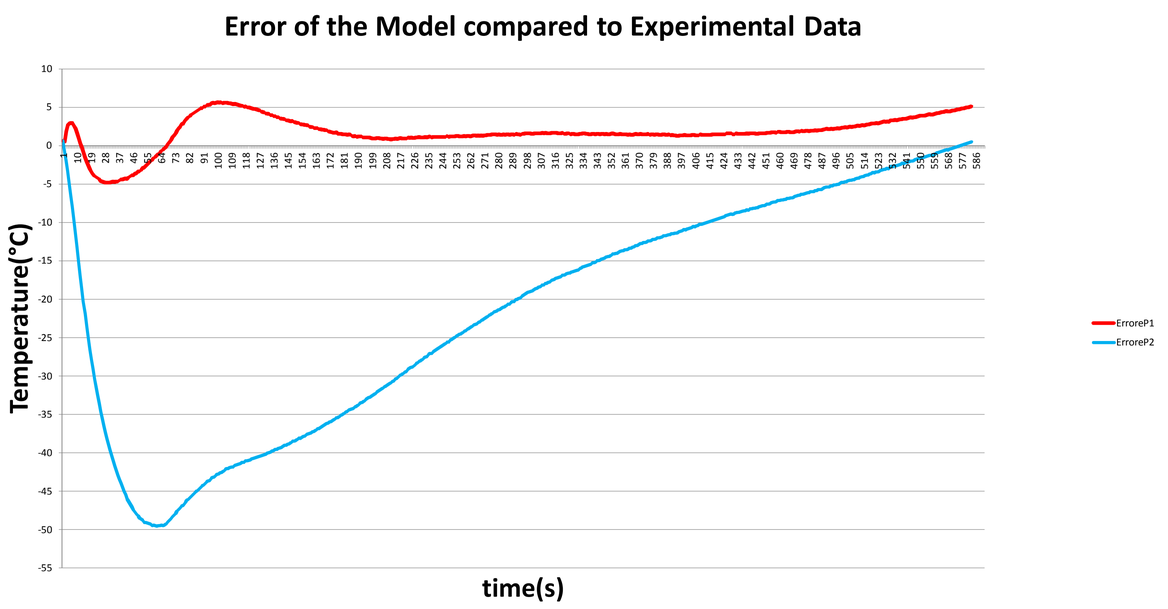

Figure 2. Internal temperature of the bottles: a comparison between the simulated functions of temperature and experimental data.

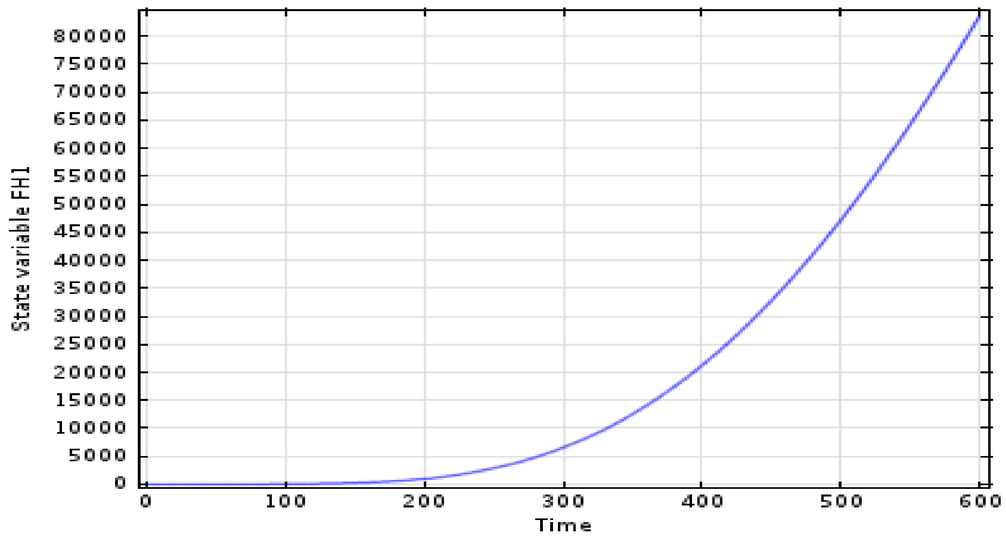

Figure 3. The simulated FH function.

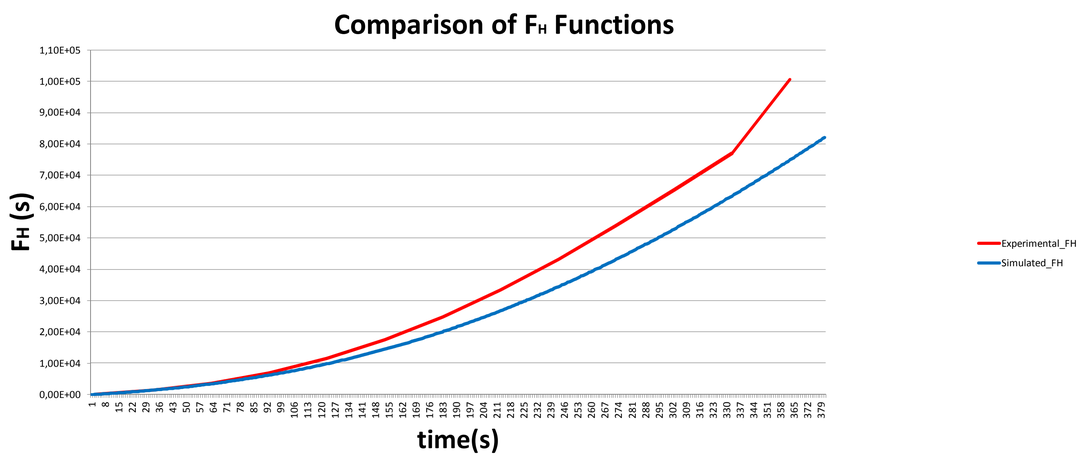

Figure 4. F_H functions: note that the experimental F_H is uniformly greater than the simulated F_H.

Conclusions: Our initial hypothesis, according to which the real physical model could be replicated with satisfactory approximation, has been fulfilled.
The FEM simulation model is very useful for a priori analysis of the feasibility of the projects.
Possible future developments are directed towards the refinement of the study and the inclusion in the model of other boundary conditions that may make it even more faithful to reality.

References:

1. R.B. Bird, W.E. Stewart,E.N.Lightfoot, *Transport Phenomena*, John Wiley and Sons (2002).
2. G. Tsuji, S. J. Harrison, *Dry-Heat Destruction of Lipopolysaccharide: Dry-Heat Destruction Kinetics*, Appl. Environ. Microbiol. **36**: 710-714 (1978).
3. A G. Tsuji, A. R. Lewis, *Dry-Heat Destruction of Lipopolysaccharide: Mathematical Approach to Process Evaluation*, Appl. Environ. Microbiol. **36**,715-719 (1978).