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Freezing water simulations in isochoric systems – preliminary analysis

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1. INTRODUCTION

Constant volume (isochoric) study at negative temperatures for different type of liquids become in the last period very interesting by the point of view of different industries. For medicine, food preservation or tissue preservation it become very important to develop new ways of preservation, because in many cases the traditional, isobaric perseveration reached his limits and we can't preserve for long periods biological matter, without a change of his molecular structure. Theoretical studies suggest that isochoric preservation could be an alternative for isobaric preservation [1-5]. A COMSOL based numerical scheme was used to simultaneously calculate the thermal stress and phase change of water in an isochoric (constant volume) reactor. The intention is to use this preliminary analysis to create a more elaborated study, time dependent, that includes temperature evolution, mechanical stress, thermal stress and phase change with pressure increase inside the reactor. The simulations in this preliminary work are intended to indicate the advantages of isochoric freezing. Basically, our intention is to show that inside a constant volume reactor filled with water, immersed in a cooling bath at a negative temperature the water freezes partially. Obviously, this is an early stage numerical study and much more theoretical and experimental research is needed.

2. MATERIALS AND METHODS

The concept of isochoric preservation is simple, and the system consist of a cooling bath, a microreactor with a pressure transducer and a data acquisition software on a PC. The temperatures and pressures are recorded using the dedicated software, that comes with the pressure transducer and the cooling bath, respectively.

For our simulations we used a theoretical 316 stainless steel 57 mL microreactor, with an internal diameter of 30 mm, outer diameter of 50 mm and an internal height of 80 mm.

The nominal conditions, a view are presented in Figure 2. Initially in the isochoric reactor we have liquid water at ambient temperature and atmospherically pressure.

Then, if we lower the temperature from the exterior using a cooling bath or any other method, the water will start to freeze, but if we look at the thermodynamic behavior in the phase change diagram of water (Figure 2) at temperatures above the triple point in the system we expect to have a certain percentage of ice I and the rest to be in liquid state.

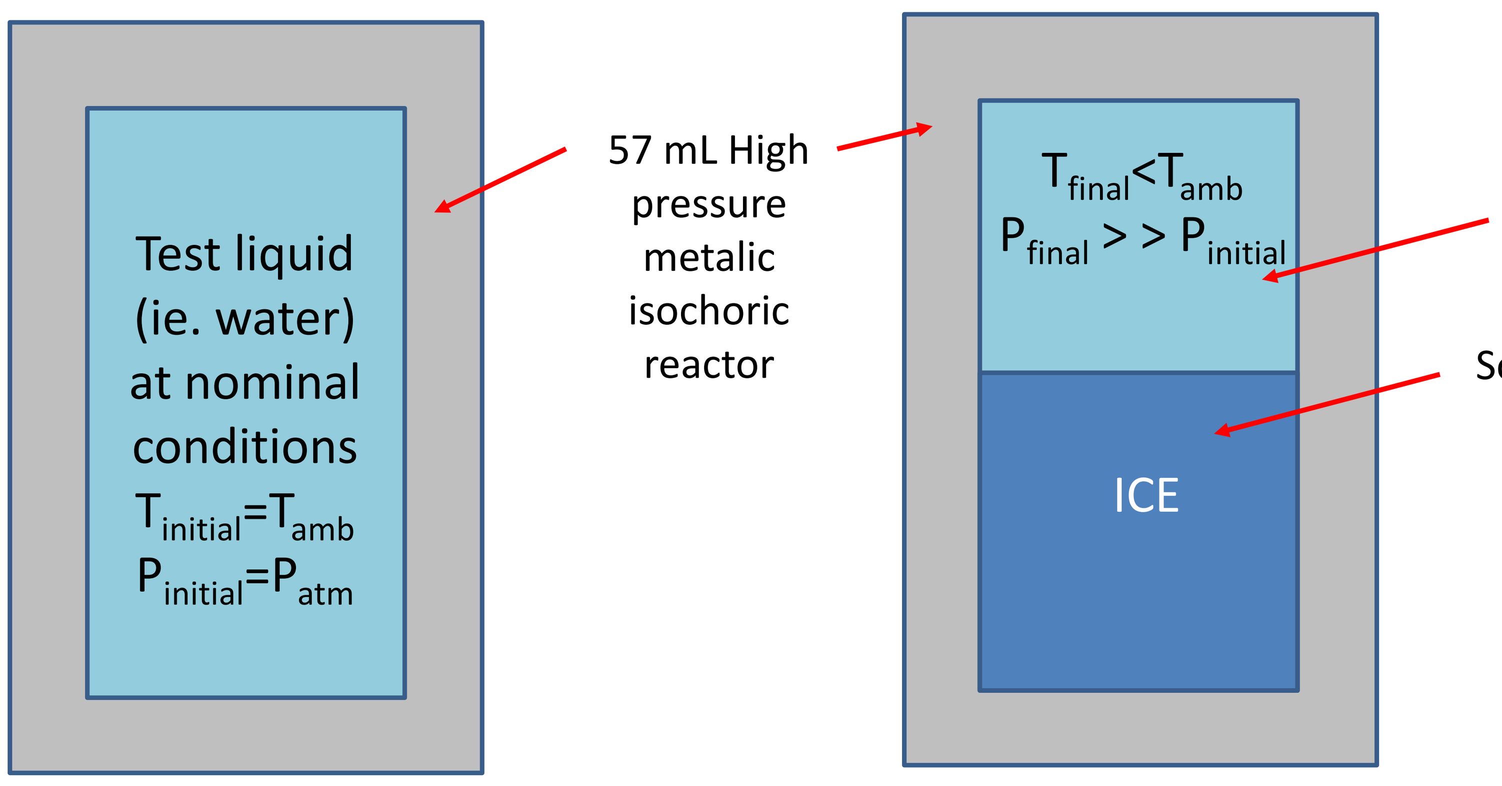


Figure 1 – Nominal conditions (left) and expected behavior inside the reactor when the isochoric reactor is immersed in a cooling bath at a negative temperature (right)

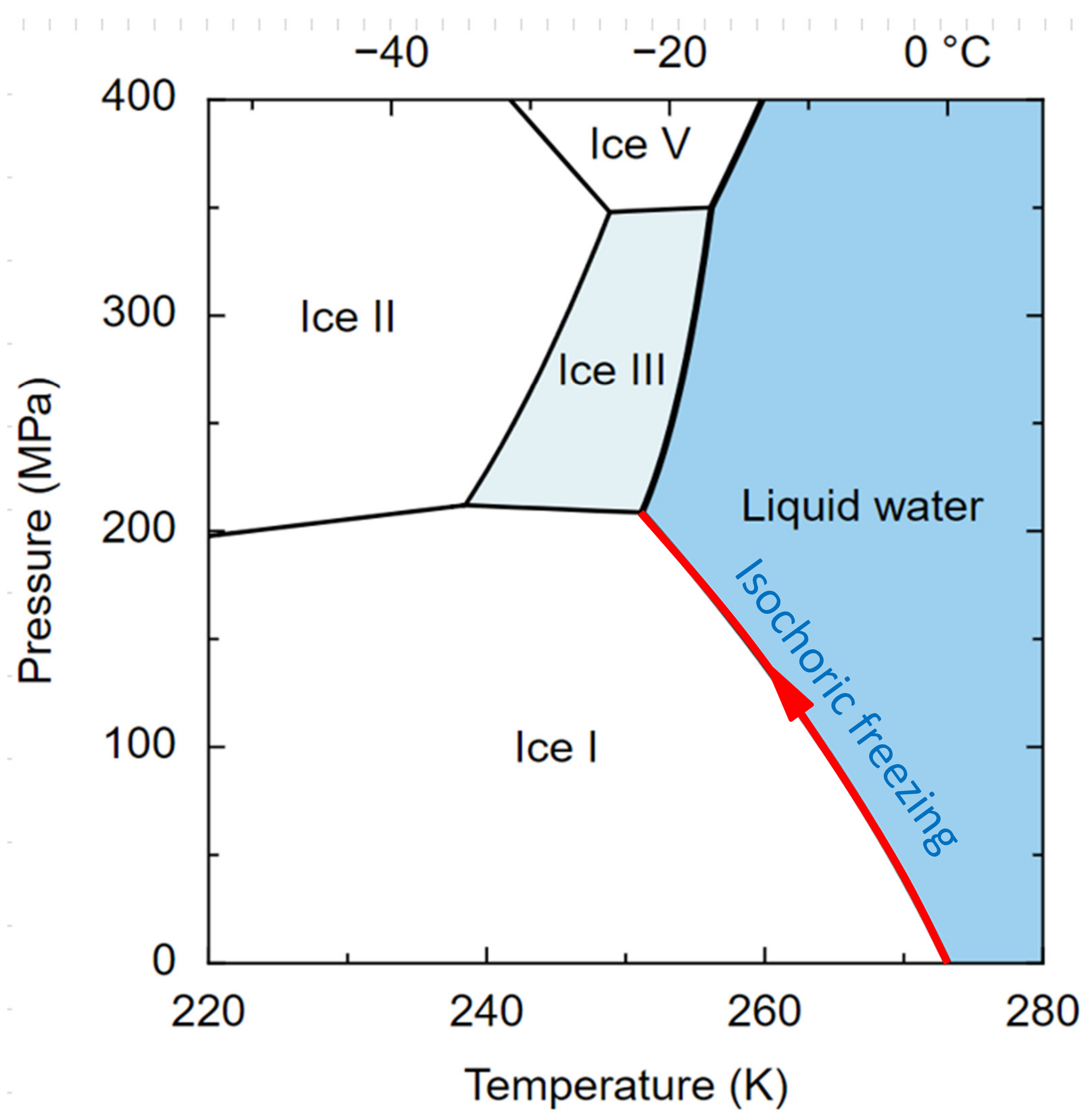


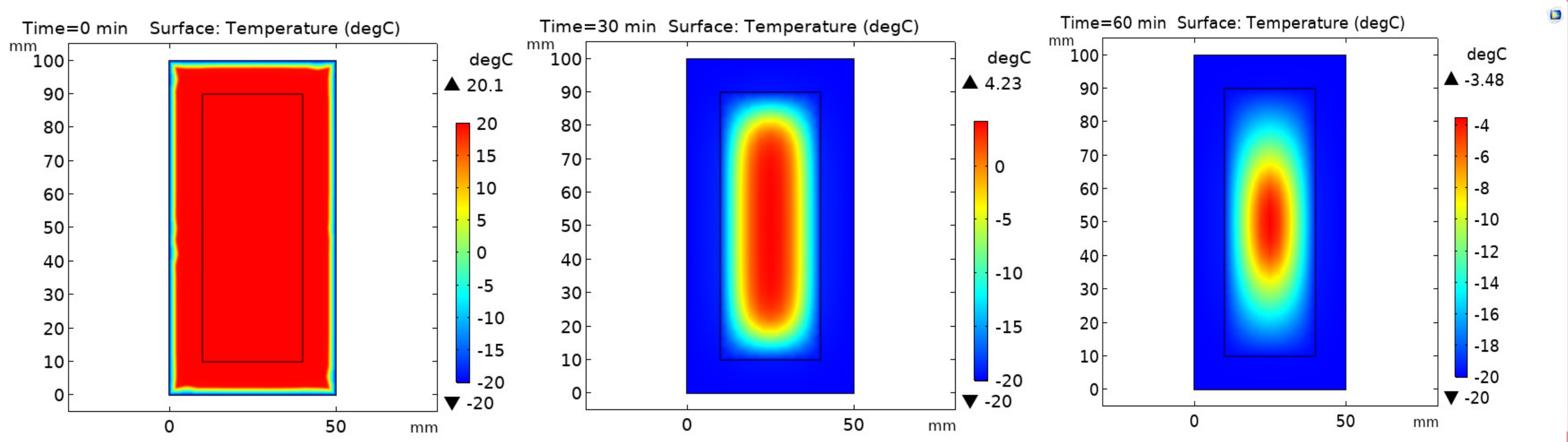
Figure 2 – Isochoric freezing processes on the phase change diagram of water

The initial temperature considered in this analysis was room temperature (20°C), the final temperature in the cooling bath was considered -20°C and the total time of immersion was 140 minutes.

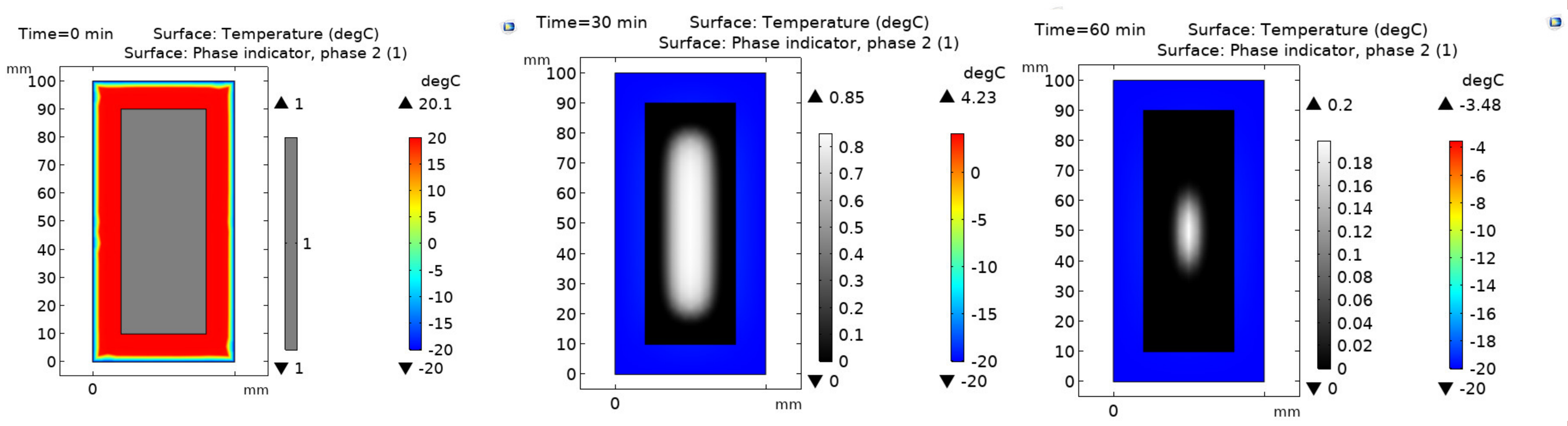
For the simulation in this study we used a 2D space dimension, Heat transfer in Solids physics from the Heat Transfer module and Thermal Stress, Solid physics from the Structural Mechanics module included in COMSOL Multiphysics simulation software.

3. RESULTS

We expect the heat transfer in the 316 stainless steel reactor to be fast and when the heat transfer starts from the stainless steel to the water, we have a moderate temperature evolution. After 30 minutes (Figure 3b), the reactor reached the temperature of the cooling bath (-20°C), but the water inside has an average temperature of -6,67°C. The water passed from liquid to ice, but after the first 30 minutes in the reactor we still have 26.23% of liquid. After 60 minutes of constant expose to -20°C (Figure 3c), all the domain is on the negative field of temperature. As we observe on Figure 4c and Figure 6, over 99% of the water has turned into ice I.



Figures 3 – Heat transfer in solid and liquid at the beginning (a), after 30 min (b) and after 60 min (c)



Figures 4 – Phase change indicator and temperature of the reactor at the beginning (a), after 30 min (b) and after 60 min(c)

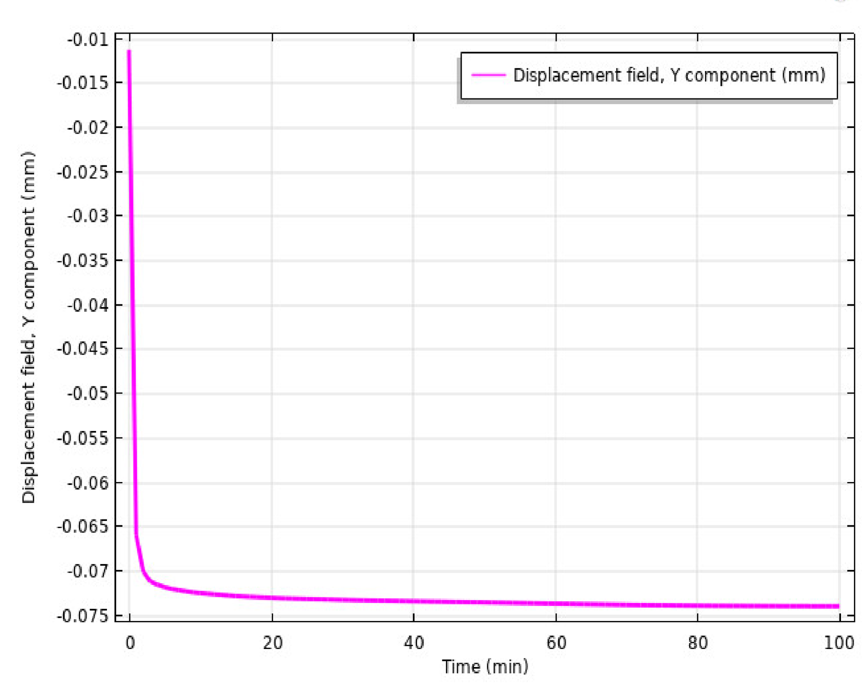


Figure 5 – Total displacement of the superior part of the reactor on Y direction [mm]

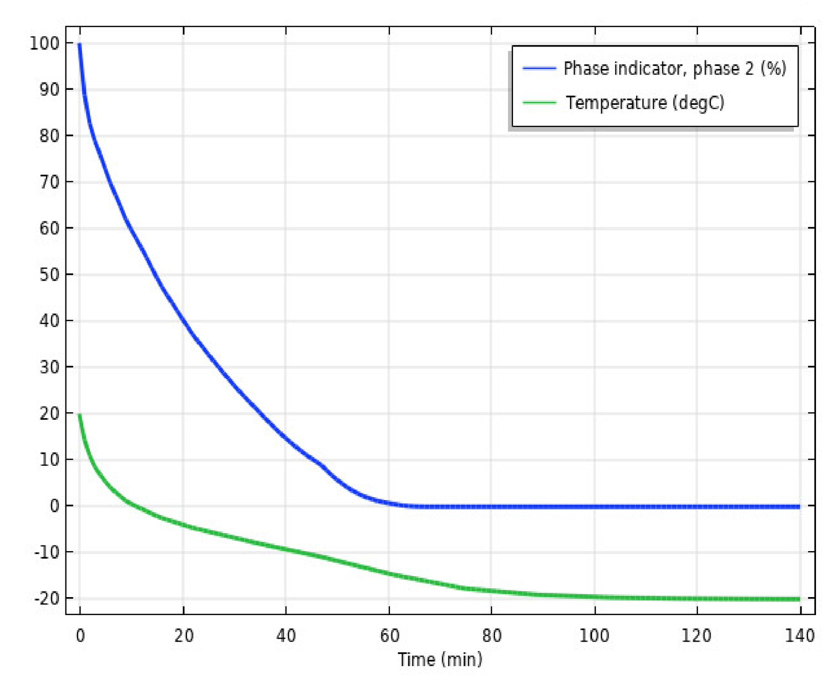


Figure 6 – Phase indicator [%] and temperature values [˚C]

The percentage of ice I formed during the freezing is in inverse proportion with the temperature, so as the temperature become lower, the quantity of ice increases (Figure 6) The total displacement of the reactor gap (on Y direction) , after 60 minutes, is around 0.075 mm. This value is not affecting results of the simulation from the heat transfer and phase transition point of view, but is important to observe the thermal stress effects on the reactor due the negative temperatures.

4. CONCLUSIONS

We consider that further studies about the behavior of the liquids in isochoric conditions are important because of the possibility of use them in different industries. A new way of conservation could be the conservation in isochoric conditions and we try to contribute on this field with our studies.

References:

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