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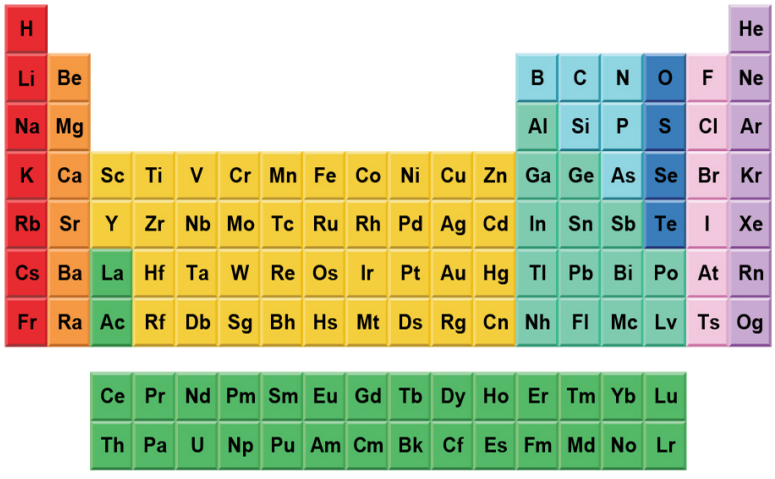
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Freezing water simulations in isochoric systems – preliminary analysis

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Abstract. Freezing liquids into ice is a complex simulation and is called a phase transformation or phase change. Isochoric (constant volume) preservation is a new thermodynamic concept that takes advantage of an until now ignored aspect of thermodynamics, life under conditions of constant volume as opposed to the conventionally studied life conditions of constant pressure. Isochoric system are simple constant volume devices, made of steel, capable of withstanding the pressures that develop in the system, with minimal deformation. Because ice-I is less dense than water, the formation of an ice nucleus in an isochoric (constant volume) chamber will cause an increase in pressure. Traditionally, ice formation is performed in an isobaric process (constant pressure) at 1 atm, because this is our natural environment and it is most convenient experimentally. The goal of this study is to introduce the fundamental thermodynamic principles and boundary conditions of isochoric (constant volume) simulations at low temperatures. In this analysis we intend to shows that homogeneous ice nucleation can be thermodynamically improbable in an isochoric system.

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 is very important to develop new ways of preservation, because in many cases the traditional, isobaric preservation reached his limits and we can't preserve for long periods biological matter, without a change of his molecular structure. For example, the human organs, collected for transplant could resist only a couple of hours with actual common accepted preservation method, but with isochoric preservation we try to find a way to extend this time to 48 or 72 hours. This means that an organ collected from a donor on any continent from the Word could be implanted to a compatible person all around the world using the current way of transport disponible for medical services.

Recent studies done on potatoes [1], fish muscle [2] or even on living biological matter [3], showed promising results for using constant volume preservation as a viable alternative [4] for isobaric preservation. The only disadvantage of using this method, is that is obvious that the intern energy of the

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system will increase (according that all liquids began to freeze at different temperatures), and because of this the inevitable formed ice will determine that in the constant volume chamber the pressure will increase. The studies done until now, led to recognition of the isochoric preservation as a pressure related cooling and freezing technique for food industry [5] and studies ongoing at the time of writing this article will develop theoretical methods of using this type of preservation for other interested industries. Every liquid solution has a different behavior and it is early to estimate for each used type a common accepted theory.

Different types of aqueous solutions can be used to preserve in constant volume conditions, but it is important to try with the most common used liquids. One of that is the water (H_2O).

The behavior of the water under isochronous conditions was well established already, and we could use it as thermodynamic and mathematic verification of the experimental data we collect, to explicit our systems [6].

With the data sets and the theoretical calculations, using Comsol software, we created a model and we start to simulate the same conditions.

2. Experimental model

The isochoric freezing system is a simple constant volume chamber capable to resist to the pressure from the inner of the reactor, with minimal deformation. The chamber is instrumented with a pressure transducer.

The isochoric chamber is a 2 mL 316 stainless steel micro-reactor MS-1 with maximum working pressure of 60,000 psi and a total of inner volume of 3 ml. The micro-reactor is capable to resist at liquid nitrogen temperatures. The inside diameter is 3/16’ and the outside diameter is 9/16’. Inside depth is 4’ and outside length is 7’. The microreactor is connected to a HP1100 0±4000 bar pressure transducer, connected to DATAQ Instruments Hardware Manager to a laptop.

The micro-reactor is filled with water and immersed in a water–ethylene glycol bath (50/50) cooled by means of a Lauda RE 1225 S cooling system (LAUDA DR. R. WOBSER GMBH & CO. KG, Lauda-Königshofen, Germany). This device can control temperatures to -25°C.

With this protocol, we are able to read the temperature from the inside of the bath (assuming that for temperature we set -20°C and the pressures from inside the microreactor. Some of the collected data sets, are presented in the tables below. We exemplify only the sets interested for our simulations.

Table 1. Time – Average temperature

Time [min]	Avg. temp [°C]
0	19.99
30	-6.67
60	-14.21
90	-19.56

Table 2. Pressure – Average temperature

Pressure [bar]	Avg. temp [°C]
0	19.99
776	-6.67
1475	-14.21
1905	-19.56

3. Theoretical model

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 1'. Initially in the isochoric reactor we have liquid water at ambient temperature and atmospherically pressure. We assume that the volume difference between the chamber we used for measurements and the chamber we used to simulate, did not affect our results.

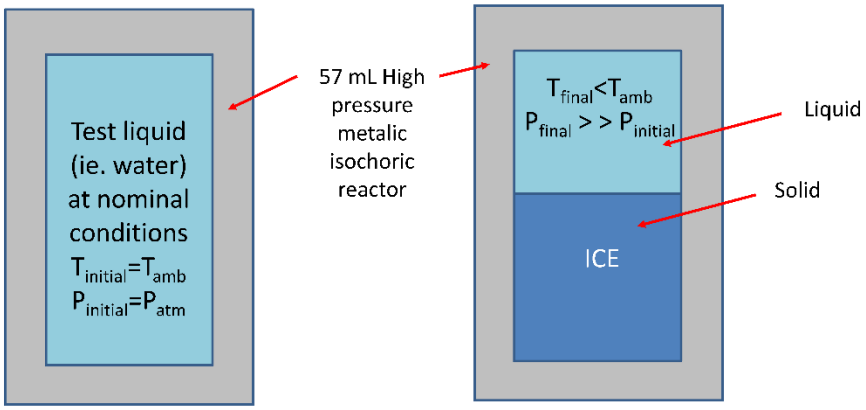


Figure 1. Initial conditions (left) and expected behaviour of water in isochoric conditions (right).

The expected behavior of water is well known under big pressures [7] and the translation to isochoric model (which has the same pressure conditions and newly introduced "constant volume" model) is also know [8] and the theoretical and experimental graph it is shown in figure 2.

The triple point of the water in isochronous conditions is at -21.985°C and 209.9 MPa. The interval for this test is below the triple point, so theoretically we will have water and ice in our system together during all measurements.

For the temperature sets tested our expectation is that not all the water will freeze during the simulations and we will have a pressure increase. However, we could simulate the displacement of the theoretical model, to see if its value affects our measurements. According that the reactor is made from Stainless steel 316 and the manufacturers data sheet provided, the expectation is that the change caused by the heat transfer and the pressure increase it will be minimal. With all these correlations we could have a real expectation for the behavior of our model during the simulation.

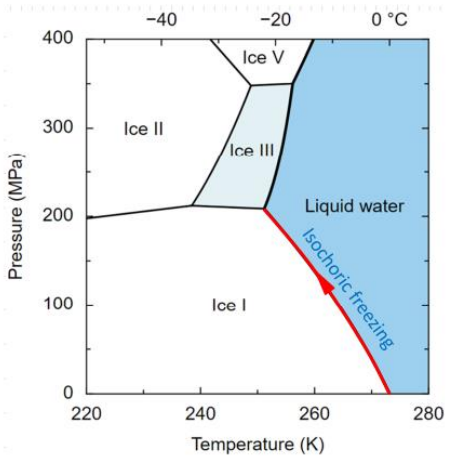


Figure 2. Phase change diagram for water under isochronous conditions.

4. Comsol simulations

We implemented the model presented in figure 1 in Comsol Simulation Software. According this our model is a cylinder, we used 2D Axisymmetric Geometry. Our problem uses coupled physics. First of all, we need Heat Transfer in Solids because we want to see the behavior of our solid and liquid part of the model during the freezing process. Also, we want to see the possible deformation of the cylinder meantime, so we need to use Solid Mechanics. Because we need to study the behavior of our system in a certain period of time, we need to use a Time Dependent Study. The difference between this type of study and a Stationary study is that the software allows us to see the transient steps of the simulation. With these two types of physics, we consider that our problem could be explained.

The exterior conditions are set as boundary conditions of temperature. On the water inside, we set the Phase Change temperature at 0°C. The total phase change interval was set from 0°C to -21.985°C.

For simplicity we used 3-time steps in our captions to exemplify the what the simulation shows us.

The initial time is "0" (figure 3a). The heat transfer started from cooling bath to the reactor. We could see and compare it from the different colorization of the steel part of the reactor.

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. After 60 minutes (figure 5c) all of our domain is on the negative field of temperature (below 0 °C)

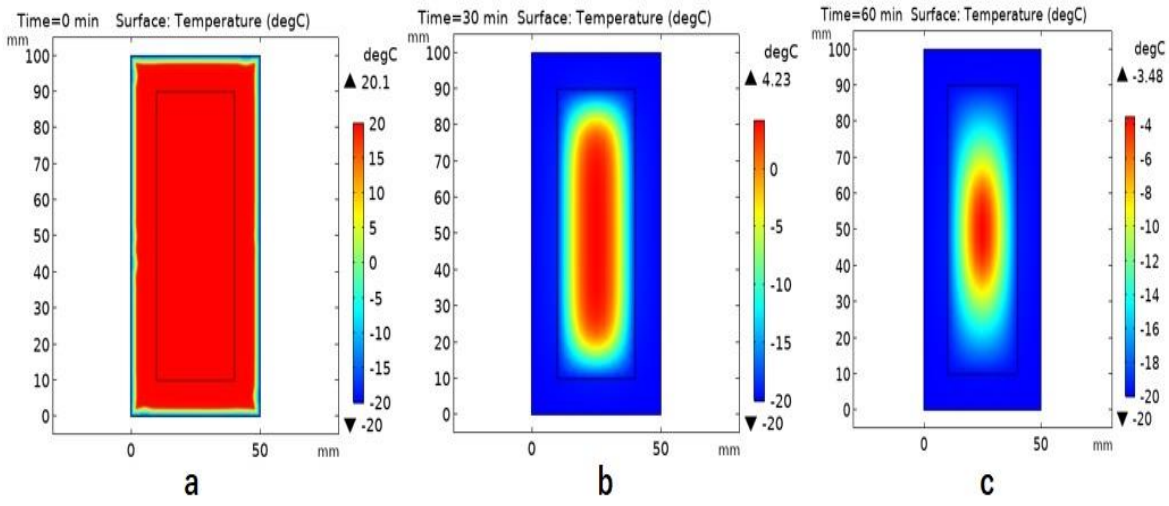


Figure 3. Heat transfer in solid and liquid at the beginning (a), after 30 min (b) and after 60 min (c).

If we are looking to the phase change, in the same time steps. At moment "0" (figure 4a), it is obvious that is impossible that the water starts to freeze, because the cylinders inner side has a temperature of 20°C. The water started to pass from liquid to ice, but after the first 30 minutes in the reactor we still have 26.23% of liquid (figure 4b). After 60 minutes of constant expose to -20°C figure 4c, just a small amount of water remains in liquid form. That is because of the set temperature for phase change is -21.985°C, so the results look correct. Simulation done for a longer period of time, shows that after 60 minutes, the system reached an equilibrium a further data to present is not relevant for this preliminary analysis.

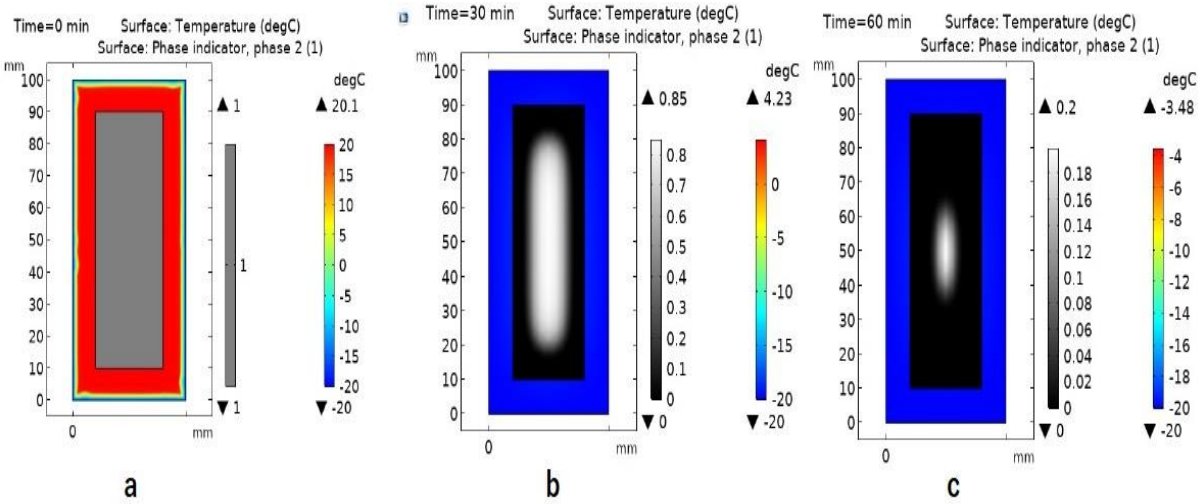


Figure 4. Phase change indicator and temperature of the reactor at the beginning (a), after 30 min (b) and after 60 min(c).

With this two sets of data, we generated a graph (figure 5). 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. After 60 minutes, we could see that our system reached an equilibrium, and the quantity of ice from the inside of the reactor remains constant.

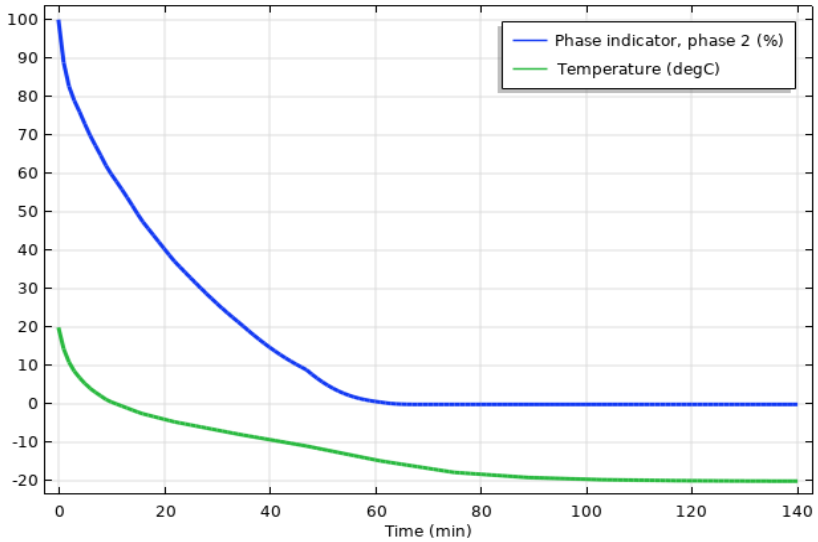


Figure 5. Phase indicator [%] and temperature values [˚C].

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 (figure 6).

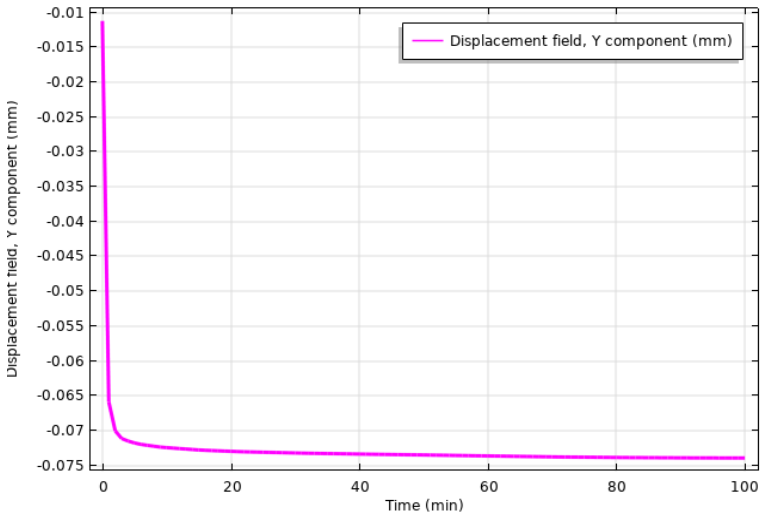


Figure 6. Total displacement of the superior part of the reactor on Y direction [mm].

5. 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. This type of conservation was recently recognized as a possible way to preserve in food industry [8], so the first steps all already done for using it on bigger scales.

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