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FEM-simulations of Tailored 3D Pressure Fields for US-assisted Oleogel Crystallization

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***Abstract* — Due to their high content of unsaturated fatty acids and controllable mechanical properties, oleogels show promise as a replacement for traditional fats in food products. Controlling the oleogel formation with ultrasound makes it possible to tune the mechanical properties of oleogels, e.g., improving their structural stability and/or mouthfeel. We previously demonstrated tuning of mechanical properties of oleogels by ultrasonic standing waves (USW) in a closed chamber. Our previous USW chamber only allowed 1D control of the pressure field. To properly tailor the oleogel properties, a more sophisticated chamber design and pressure field control technique is required. A new design for USW chamber and the frequency-domain time-reversal technique for field control were studied via simulations. We show that the proposed technique can create tailored USW fields inside a chamber filled with oil. Further, we show results of particle tracing simulations, and compare the idealized model with realistic phased arrays of transducers, to determine the requirements for the arrays to achieve a suitable resolution for shaping the field.**

Keywords — FEM, piezoelectricity, phased arrays, digital twin, food science, edible metamaterial

I. Introduction

Oleogels are lipid-based materials, having a 3D structure of molecules, referred to as oleogelators, giving them rigidity. Due to their high content of unsaturated fatty acids and controllable mechanical properties, oleogels have shown promise as a replacement for traditional saturated fats in food products [1].

By controlling the location of oleogelators during the crystallization process, it is possible to tune the mechanical properties of oleogels, e.g., improving their structural stability and/or mouthfeel. Control of oleogel crystallization by ultrasonic standing waves (USW) was previously shown [2]. In previous studies the USW control was limited to use of plane waves, driven with single large piezoelectric transducer, only allowing 1D control of the oleogelators' position. Having the USW chamber instead surrounded by a phased array of transducers (PAT), one can achieve 3D control of the oleogelators, allowing the production of tailored oleogel crystallization patterns.

The feasibility of the described method was studied with simulations, before constructing an experimental test setup. The next sections describe the proposed method for controlling the acoustic field and show results of creating two kinds of patterns within the USW chamber. Feasibility of the method is assessed by studying the requirements for PAT necessary to achieve a suitable resolution for shaping the field.

II. Methods

Time-reversal (TR) is a technique that can be used to focus acoustic waves [3]. The technique is based on the reciprocity principle of the wave equation [4]. Traditionally TR is done in time domain, but the same principle also works in frequency domain [5].

In frequency domain time-reversal (FDTR) the forward propagated signal is first transmitted from the source located at the desired focus point and then recorded by transducers placed around it (Fig. 1A). In the back propagation phase the complex conjugate of the recorded signal is transmitted back by the transducers, causing a pressure anti-node to form in the original source location (Fig. 1B).

In addition to focusing the acoustic field only to a single location, the FDTR method may also be applied to recreate more complex shapes. The feasibility of using the FDTR method to create a tailored 3D pressure field was studied using simulations. Two versions of the simulation model were made. Model 1 with transducers modelled as ideal point sources (Fig. 2A), and model 2 with transducers modelled with finite sized pressure sources on three sides (Fig. 2B). The number of PAT surfaces in model 2 was limited, as it was deemed unrealistic to completely surround the USW chamber with transducers.

Simulations were made using a commercial finite-element method (FEM) modelling software COMSOL Multiphysics® (version 6.0). Modelling the acoustic fields was realized with the *Pressure Acoustics, Frequency Domain* physics interface and the particle tracing was simulated using *Particle Tracing for Fluid Flow* interface. Frequency domain simulations were conducted with 1 MHz frequency, with the wavelength in oil being 1.48 mm.

Both simulation geometries consisted of a cube shaped chamber, with sides of 1 cm length. In model 1 the point sources were positioned in a regular grid with 0.5 mm spacing (Fig. 2A). In model 2 the transducer elements were spaced on a regular grid with an adjustable element and pitch size (Fig. 2B).

The chamber walls had *Impedance* boundary conditions. On the topmost wall the impedance was set to represent an air-oil interface and on the other walls the impedance was set to represent a plastic-oil interface. Pressure sources inside the chamber were introduced by drawing the desired shape of the pressure anti-nodes into the geometry and assigning a pressure source condition on the drawn shape.

Two kinds of shapes were created using the FDTR method: A regular shape consisting of rectangular cells, and a helicoidal shape in the middle of the chamber. The rectangular shape was selected as constructing similar regular shapes allows creating oleogels with isotropic mechanical properties, which can then be tuned by changing the dimensions of the internal structure. The helicoidal shape in turn was chosen to show that the method also can create non-regular, anisotropic shapes.

During the forward propagation phase the internal pressure source condition was set to 'active', whereas the transducer pressure sources were disabled. During the backward propagation phase, the internal sources were disabled, and transducer sources were activated. Transducer pressure sources used the complex conjugate of the average forward propagation pressure as their pressure condition.

A particle tracing simulation was done by simulating the movement of 10000 monostearin particles released in the oil. With the particle tracing simulation, the aim was to visualize the areas where oleogelators mostly accumulate. As only the final locations of the particle accumulation were of interest for this study, the fluid viscosity was artificially scaled up during the particle tracing, to improve the stability of the simulation.

To map the requirements for the realistic PAT, a series of simulations was done with varying array element size. A model with 0.8x0.8 mm^2 elements was used as baseline, and the size of the array was scaled up to determine the upper size limit. Typically, the minimum element size for PAT is 0.2 mm [6].

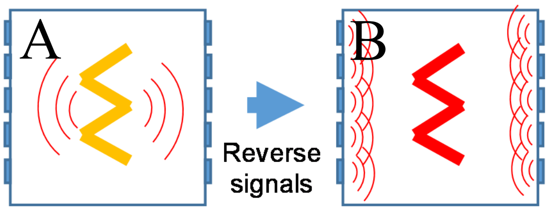

Fig. 1. Illustration of the time-reversal method. A: Forward propagation phase. Pressure source in introduced inside the chamber, surrounded by listening transducers. B: Back propagation phase. Reversed signals are transmitted back using the same transducers, forming the initial shape inside the pressure field.

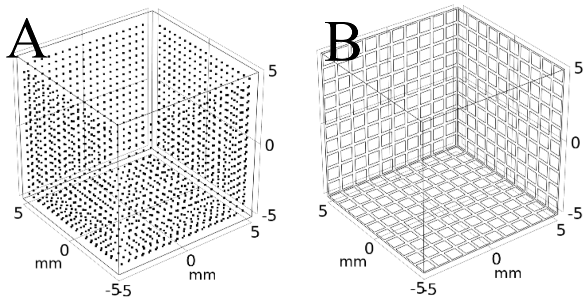

Fig. 2. Simulation geometry. A: Geometry with transducer elements as ideal point sources on all sides but the top. B: Geometry with realistic PATs on three sides of the chamber.

III. Results and Discussion

Fig. 3 shows the pressure fields during the forward propagation phase for both the rectangular and helicoidal initial shapes. In Fig. 3A, line sources arranged in a rectangular pattern were used as the pressure source, whereas in Fig. 3B, a helicoidally arranged pressure source was used. Results of this simulation step were used as the basis for the FDTR process during the back propagation phase.

Fig. 4 shows the results of the back propagation phase with the ideal simulation model (Fig. 2A). Figs. in the left column (Fig. 4A, C, E) show the results for the rectangularly shaped case, whereas the right column (Fig. 4B, D, F) shows the results for the helicoidal shape.

Figs. 4A, B show the back propagated pressure field. The field shape mimics the initial pressure field of the forward propagation phase (Fig. 3A). Figs. 4C, D visualize the node locations withing the pressure field. In Fig. 4D the anti-node areas are plotted for improving the readability of the field. Fig. 4E, F show the particle locations in the back propagated pressure field. In Fig. 4F the front half of the solution is hidden, to allow one to observe the order of particles within the field. A similar but tilted field, expanding in the opposite direction is observed when the back half of the solution was hidden.

Fig. 5 shows the pressure field created during the backward propagation phase with the model shown in Fig. 2B. With 0.8 mm array elements (Fig. 5A, C), the field shape is comparable to the field created with the ideal model, even if it shows some minor differences. Raising the element size to 1.6 mm (Fig. 5 B, D) cause distortions to the pressure field.

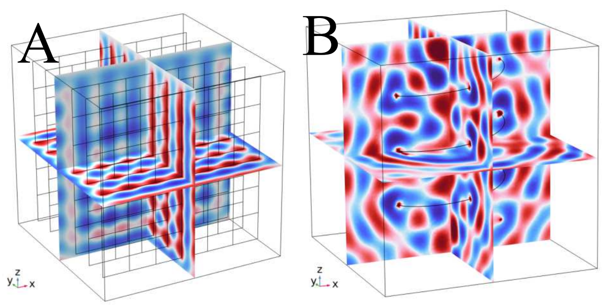

Fig. 3. Pressure field during forward propagation phase. A: Rectangularly shaped pressure sources. B: Helicoidally shaped pressure source.

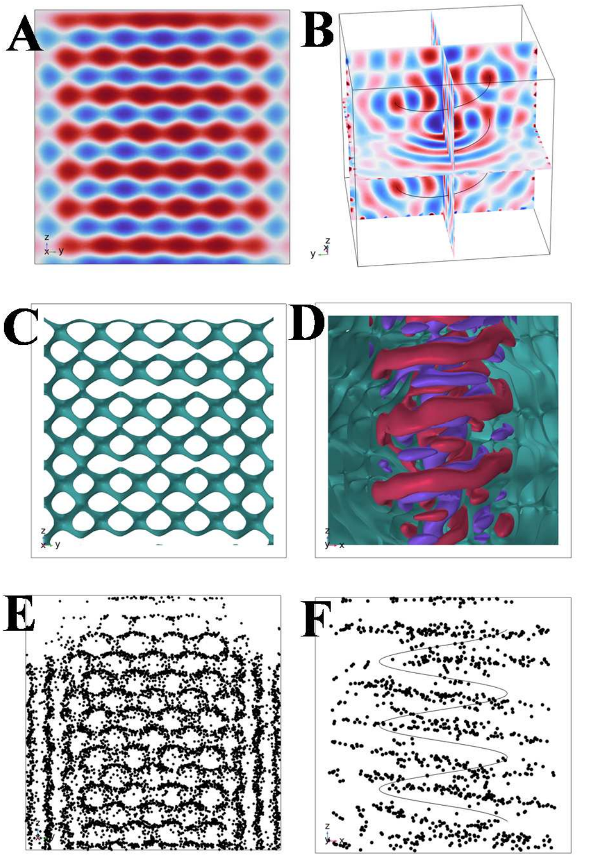

Fig. 4. Results of back propagation. A, C, E: Pressure field, pressure nodes, particle tracing, in the case with rectangular sources during forward propagation. B, D, F: Pressure field, pressure nodes and anti-nodes, particle tracing, in the case with helicoidal source during forward propagation.

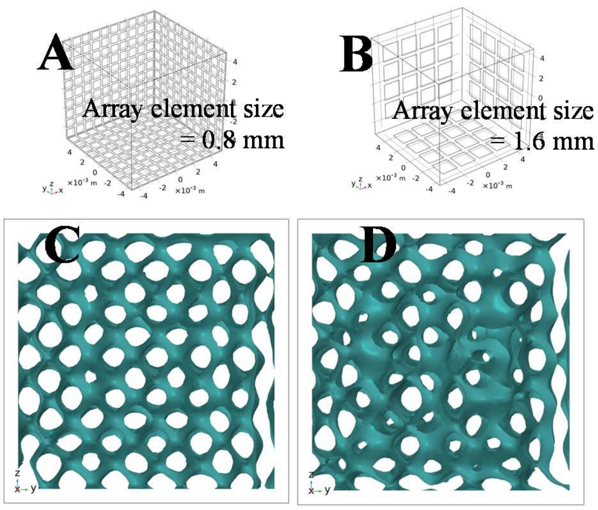

Fig. 5. Results of back propagation with realistic PATs. A, C: Simulation geometry and pressure nodes with 0.8 mm element size. B, D: Simulation geometry and pressure nodes with 1.6 mm element size.

The simulation forecasts provide a basis for follow-up experimental work, where a simulation-to-experimental TR [7,8] could be applied for creating the tailored pressure fields. Having a detailed simulation model of the oleogel chamber and the PAT could allow directly linking simulations and experiments, allowing the use of simulated signals for the real-world setup.

Alternative methods for achieving 3D field control could be by employing acoustic holograms instead of PATs [9]. In principle such a method could allow similar control of the field as FDTR, but with traditional transducers. With PATs one could employ different optimization algorithms to solve the phase delay for each array element [10]. However, such optimization methods often struggle to consider reflections from the environment, which is required with USW chamber.

IV. Conclusions

Based on our results, FDTR appears to be a possible method for controlling the oleogel crystallization process. Fig. 4 shows that FDTR can manipulate the pressure field, allowing to control the location of the oleogelators during the process.

Further, the method appears to work when using realistic PAT (Fig. 5A, C), given that the element size is < 1.6 mm with 1 MHz frequency. As the PAT element size decreases, the cost of PATs increases rapidly, making it of interest to determine the upper limit of the element size for FDTR process.

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