Evaluation of Faraday instabilities in small vessels

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1. Introduction

Different sort of problems arise from sloshing liquids in containers. Well studied examples include the damage that earthquakes can have on dams, water reservoirs and oil tanks, or the displacement of fuel inside the tanks of jet planes and space rockets [1]. Mechanical stress in agitating biological or pharmaceutical liquid solutions can result in denaturation and aggregation, thereby affecting the stability of the products profoundly. In fact, biomolecules have a high propensity to undergo physical instability reactions that are encountered by changes in the three dimensional structure of the active ingredient [2]. One important aspect to understand the agitation of aqueous solutions is the stability threshold above which the free surface shows normal modes. Under vertical vibration of the vessel, these modes are stationary and can grow large in intensity. Therefore, they can induce a high shear stress on the solved molecules.

OpenFOAM allows a detailed study of the agitation of a liquid inside a vessel. The two-phase system can be studied with a transient solver in an accelerated frame. The agitation profile can be set to sinusoidal to study in detail the stability threshold or multi-harmonic for testing realistic agitation profile. By monitoring the wave height and the mode composition, the induced instabilities can be characterized.

In this work, OpenFOAM simulations of a liquid in contact with air will be performed to study the Faraday instability threshold. The simulations will be compared to a semi-analytical theory [3] and to experiments done on a vertical vibration table. The main consequences for the stability of the liquid confined in the vessel will be discussed.

2. Methods

2.1. OpenFOAM simulations

The simulation of two incompressible and immiscible fluids is done with the *interFoam* solver. It uses the Volume of Fluid (VOF) phase-fraction approach to describe the interface and includes gravity effects. The fluids, water and air, are enclosed in a cylindrical vessel. Two types of geometries have been defined to solve the problem. One is a 2D rectangular domain with an axisymmetric axis and two wedge boundaries. The other contains a full 3D model of the cylindric container. Hexagonal structured meshes have been defined in both cases, with a finer grid in the central part for a better definition of small movements of the water surface. The simulations have been run first using a 2D axisymmetric geometry. The zones of interest have been checked more carefully with the full 3D model to discard any possible artifact coming from the breaking of the axial symmetry.

The two phases are initialized in the gravitationally stable configuration. The vertical vibration is studied in the reference frame of the vessel and it consists of a constant gravitational term and an oscillating term

$$A(t) = -G + A_0 \cos(\omega t) \tag{1}$$

A_0 is the acceleration amplitude and $\omega = 2\pi f$ the angular velocity. The acceleration amplitude and the frequency value are included as parameters in the *constant/* folder. The dynamics of the free surface is governed by the surface tension $\sigma = 0.072\ N/m$. The viscosity effects at the walls and the interface have a significant influence on the normal modes but it does not change the main characteristics of the instability [4], therefore only bulk viscosity effects have been included.

The postprocessing has been automatized by calculating the wave height after each time step from the alpha field. The wave height is defined as the height difference between the minimum and the maximum vertical values of the *alpha* field isosurfaces. Each simulation has been run for until the instability forms. Then, the wave height data is collected during $5 - 10$ periods. Acceleration between $0.1G$ and $1G$ and excitation frequencies ranging from $3\ Hz$ to $150\ Hz$ have been studied.

The cases have been submitted to the online HPC platform *KaleidoSim*, which provides virtual machines with up to 96 cores for OpenFOAM users. The platform, currently in the test phase, will be soon open for any user. Its main feature is that a large number of jobs can be submitted simultaneously.

2.2. Experimental methods

A vial has been filled with water. The mass density and viscosity of the fluids are shown in Table 1.

	Mass density (Kg/m³)	Dynamic viscosity (mPa·s)
Water	1000	1
Air	1.146	0.0172

Table 1.- Mass density and dynamic viscosity of the two fluids.

The vibration experiments were conducted in a Lasmont Field-to-Lab® table sized 1000 Vibration Testing System which performs harmonic and random vibration tests in the 1-300 Hz frequency range and maximum peak-to-peak amplitude of 10.2 cm. A hydraulic actuator and a hydraulic power supply drive the vibration system. The parametric excitation has been studied by performing a frequency scan from 5 Hz to 120 Hz with 2 octaves at constant accelerations (0.1G, 0.18G, 0.32G, 0.56G and 1.0G, where G=9.81 m/s²). The free surface of the vial has been recorded with a Mikrotron MotionBlitz EoSensR high speed camera equipped with a complementary metal–oxide–semiconductor (CMOS) sensor that can record up to a maximum of 506 frames per second (fps) at 1280x1024 pixel and a 8-bit monochrome resolution. The vibration test has been recorded at 25 fps in a single movie.

The movie has been imported and processed frame by frame in MATLAB®. First, the vertical vibration movement has been subtracted by aligning the bottom of the vial in all the frames. By calculating the frame-to-frame geometric difference Δ_i between all the pixels of two subsequent frames,F_{i-1} and F_i , the change in the position of the water can be followed

$$\Delta_i = \sqrt{\sum_{j=1}^{N} \frac{\left([F_i]_j - [F_{i-1}]_j\right)^2}{N}} \tag{2}$$

The effect from small changes in the frame coming from other sources (illumination, record noise…) has been estimated by calculated Δ_0 while the liquid was in rest and it has been subtracted from Δ_i. More details about the experimental methods and data analysis strategy can be found in reference [5].

2.3. Stability analysis

The stability of the free surface of a fluid in contact with air and inside a closed vessel has also been studied using a Floquet stability analysis. In its initial state free surface is perfectly horizontal. For small waves, the position of the free surface can then be assumed to be located at z=0. This will define reference position for the vertical axis and the rest state. For small velocities and deviations from the flat surface, the Navier-Stokes equations can be linearized

$$\partial_t \vec{U}_i = -\frac{1}{\rho_i}\vec{\nabla}P_i + \frac{\eta_i}{\rho_i}\nabla^2\vec{U}_i + A(t)\hat{z} \quad (3)$$

Where the velocity is vertical $\vec{U}_i = U_i\hat{z}$ and the the hydrostatic pressure is decomposed from the total pressure $P_i = -\rho g h + p_i$. The non-slip boundary conditions at the vertical wall define the solution in axial coordinates (r, θ, z) as

$$U_{j,z} = J_m(\lambda_{mn}r)\sin(m\theta)\,w_{j,mn}(z,t) \quad (4)$$

$J_m(\lambda_{mn}r)$ is the Bessel function of the first kind for mode (m,n) and $1/\lambda_{mn}$ is the position of its nth root. The Faraday waves are composed by modes. The allowed modes are discretized and bounded from below by $\lambda_{11} = 2.40483/r$. The solutions $w_{j,mn}$ are Fourier series

$$w_{j,mn}(z,t) = e^{(\mu+i\alpha)t}\sum_{k=-\infty}^{\infty} w_{j,mn}^{k}(z)e^{ik\omega t} \quad (5)$$

The exponent $\mu + i\alpha$ is the Floquet exponent and $i = \sqrt{-1}$ the imaginary number. Only the harmonic (α=0) and subharmonic (α=1/2) cases lead to stationary solutions. The eigenvalue problem is solved numerically and the lowest real eigenvalue A_0 is the excitation threshold for the mode at a given frequency [4]. More details about the analysis can be found in reference [5].

3. CONCLUSIONS

OpenFOAM simulations of a liquid in a small vessel under vertical vibrations have been performed for two incompressible and immiscible fluids using the *interFoam* solver. For that purpose, the standard interFoam solver has been modified to include harmonically oscillating frames. After the equilibration stage, the creation of Faraday waves has been monitored. For that purpose, a post-processing utility has been developed that records the wave height for each time step. This avoids saving the calculated fields and has improved the quality of the data analysis. The number of simulations performed has been maximized using a 2D axisymmetric domain and an online HPC platform for OpenFOAM users, KaleidoSim.

The numerical study of the stability threshold of a liquid in a small vessel under vertical vibrations has been validated using experiments and a linear stability analysis. The existence of a low stability region between 10 and 70 Hz has been confirmed qualitatively. The main source of inaccuracy in the position of the stability tongues come from the non-linear viscosity effects exerted by the container walls and the contact angle with the vessel.

The broken shape of the instability threshold makes highly non-trivial the study of agitation effects. This work is a first step to studying horizontal vibrations in vessels, where the flip-flap movement of the liquid makes the use of analytical techniques more difficult. It also shows that OpenFOAM can a valuable tool to study the stability of fluids.

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