Computational Fluid Dynamic simulation of the supersonic CO₂ expansion during champagne cork popping

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Abstract

Behind the iconic “pop!” accompanying the uncorking of a champagne bottle hides a gas flow of surprising complexity. Its modeling is made delicate by its supersonic nature, its interaction with the cork stopper, the eminently unsteady character of the flow escaping from the bottle, and the continuous change of the geometry of the computational flow domain due to the displacement of the cork. Our numerical simulations reveal the formation, evolution and dissipation of shock wave patterns during the first millisecond following cork popping. A first crown-shaped shock wave pattern develops radially, then followed by the formation of a detached shock wave, or bow shock, induced by the presence of the cork in the axial path of the supersonic gas. The numerical simulations correctly reproduce the position of the bow shock previously observed through high-speed imaging.

Introduction

Nowadays, after more than three centuries and undergoing continuous refining, champagne has undoubtedly become the most renowned French sparkling wine, praised world-wide for the fineness of its carbon dioxide (CO_2) bubbles.¹ Indeed, during champagne making, bottles reach a high pressure because gas-phase CO_2 forms together with ethanol during a key step in-bottle fermentation process promoted by adding yeasts and sugar in the bottles hermetically sealed with a cork stopper.¹ This is basic application of Henry’s law which states that the concentration of dissolved CO_2 in the liquid phase is proportional to the partial pressure of gas-phase CO_2 in the bottleneck. Moreover, because the solubility of CO_2 in the liquid phase is strongly temperature-dependent (the lower the temperature of the wine, the higher the gas solubility), the partial pressure of gas-phase CO_2 in the bottleneck is therefore also strongly temperature-dependent (the lower the temperature of the wine, the lower the partial pressure of gas phase CO_2). Otherwise, because the driving force behind the cork popping process is the force exerted by gases under pressure in the bottleneck on the base of the cork stopper, the cork popping velocity is therefore definitely under the influence of the champagne temperature, as already shown in a previous article.²

During the cork popping process, concomitantly with the cork stopper being expelled from the bottleneck under the action of pressure, a plume made of a gas mixture mainly composed of CO_2 (with traces of water vapor) freely expands out of the bottleneck through ambient air and experiences adiabatic cooling.^{3–5} High-speed video imaging was used recently to visualize champagne cork popping, and especially the condensation processes following the adiabatic expansion of the gas mixture found in the bottlenecks of transparent champagne bottles stored at different temperatures.⁵ The bottles’ temperature (and therefore their inner pressure) was found to be a key parameter concerning the condensation processes that can occur above, and inside the bottlenecks. Most interestingly, for the bottles stored at 20°C (under a pressure close to 7.5 bar), the characteristic grey-white cloud of fog classically observed above the bottlenecks of bottles stored at lower temperatures was replaced by a more evanescent plume, surprisingly blue, starting from inside the bottleneck.⁵ Depending on the strongly bottle temperature dependent saturation ratio experienced by gas-phase CO_2 after adiabatic expansion, it was emphasized

that blue haze is the signature of a partial and transient heterogeneous freezing of gas phase CO_2 on ice water clusters homogeneously nucleated in the bottlenecks.⁵ Even more recently, a comparison between the condensation phenomena accompanying cork popping from bottles stored at 20 and 30°C was made.⁶ The initial bottleneck-to-ambient-pressure ratio (7.5 for the bottles stored at 20°C, against about 10 for those stored at 30°C) much exceeded the critical ratio needed for the $\text{CO}_2/\text{H}_2\text{O}$ gas mixture to reach Mach 1, thus forming under-expanded supersonic jets expelled from the throat of the bottlenecks. Moreover, during the very first millisecond following the cork popping process, evanescent normal shock waves were unveiled in the plumes, until the reservoir-to-ambient-pressure ratio goes below a critical ratio needed for their formation, which were *de facto* seen vanishing.⁶

Actually, the expansion of a high-pressure gas suddenly opening into a low-pressure environment gives rise to a so-called free jet, as opposed to a jet confined by the walls of a duct. The free jet acquires supersonic speed when the speed of sound is reached at the outlet that separates the high and low pressure areas. This condition is met when the ratio of the upstream and downstream pressures is greater than approximately 2 (the precise value depends on the ratio of the specific heats of the gas). The free jet can then reach very high Mach numbers, which corresponds to high speeds but also to temperatures which can be extremely low, close to absolute zero,⁷ under the law of conservation of energy. This specificity of supersonic flows is used in particular to carry out studies of chemical reactivity⁸ or spectroscopy⁹ at very low temperature in the gas phase. The interaction of the supersonic free jet with the downstream static gas leads to the formation of a complex network of shock waves and boundary layers, also called diamond shocks by Ernst Mach who first described them using shadowgraphy.^{10,11} Note that at high pressure ratios, a normal shock wave forms, perpendicular to the flow, through which the gas becomes subsonic again. For a circular orifice, this normal shock wave is called a Mach disk. Such a shock wave occurs at the outlet of Laval's nozzles which propel rockets, missiles or scramjets, but can just as easily form during the eruption of a volcano,¹²⁻¹⁴ or during the formation of geysers observed on the surface of the Europa satellite.¹⁵ The Mach disk is formed all the further from the gas outlet the greater the upstream and downstream pressure ratio.¹⁶ The position of the Mach disk remains stationary as long as the upstream and downstream pressures do not change over time, which is not the case if the volume of the high pressure gas is finite, as is the case for example for experiments carried out in a shock tube¹⁷ or for gas escaping from a bottle of champagne. To simulate this type of expansion, it is then necessary both to take into account the finite nature of the high pressure reservoir¹⁸ and consider an unsteady flow. An additional difficulty in the case of the bottle of champagne is linked to the presence of an obstacle on which the flow is impacting. Supersonic flow hitting a surface leads to the formation of a detached shock wave¹⁹ through which the gas will adapt to the low speed and high pressure conditions imposed by the presence of the obstacle. This situation is very similar to the cold spray process device which consists in ejecting particles at supersonic speeds which collide with a substrate to be treated.²⁰ In this case, two shock wave systems interfere: a free jet type structure and a detached shock wave type structure. The situation is indeed quite similar during the champagne cork popping process. The gas mixture expelled from the bottleneck must adapt to the ambient pressure

through a network of shock waves but also face the presence of the cork that is in its path. Nevertheless, a significant difference from the study by Pattison *et al.*²⁰ is that the distance between the gas outlet (the bottleneck) and the obstacle (the flying cork) varies over time.

The present study addresses the aforementioned issues by considering the champagne cork popping process as a supersonic free jet expelled from a finite reservoir and impacting a moving obstacle. Based on Computational Fluid Dynamics (CFD) calculations, the shock wave structure experienced by the gas flow expelled at supersonic speeds from the champagne bottleneck after ejection of the cork stopper was followed with time. The calculation performance and the stability of the two-dimensional axisymmetric method used were evaluated by comparing the numerical results of the transient gas expansion with the normal shock wave position previously observed through high-speed video imaging.^{5,6}

Results

Shock wave pattern. According to gas dynamics and as confirmed by our simulations shown in Fig. 1, the gas escaping from the bottle reaches a supersonic regime. Before describing into details the flow field properties revealed by our numerical simulations, let's briefly recall some basics of compressible flow²¹. Two conditions have to be met by the gas flow to break the speed of sound. The first one relates to the existence of a throat, i.e. a spatial zone delimiting a converging duct area from a diverging one. Due to the mass conservation, a subsonic flow needs to move in a converging duct to be accelerated. Conversely, the decrease of density of a supersonic flow is so rapid that it cannot be compensated anymore by the velocity increase to maintain its mass flow ($\dot{m} = \rho A V$). Both velocity (V) and area (A) must increase to compensate for the density (ρ) decrease of a supersonic flow. It follows that the speed of sound can only be reached if the gas flow passes through a throat. The shoulder of the bottle of champagne behaves as a converging duct whereas the diverging one is only virtual, it corresponds to the large atmospheric volume in which the high pressure gas is "freely" discharging once the cork popped. The second condition to reach a supersonic regime is that the flow must reach the speed of sound at the throat, which then behaves like a sonic throat characterized by a Mach number equal to 1, this condition is called choked flow. In case this condition is not satisfied, the gas will decelerate downstream the throat. A choked flow is obtained provided that the gas reaches the critical pressure p^* at the throat

which is given by the isentropic choking pressure ratio $\frac{p^*}{p_0} = \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}}$, where p_0 is the pressure prevailing in the bottle and where γ denotes the specific heat ratio of the gas. Thus, a supersonic flow is developing provided that $p^* / p_0 \leq 0.5$, or equivalently, that the nozzle pressure ratio (NPR) $p_0 / p^* \geq 2$.

As the initial pressure of a bottle of champagne far exceeds two atmospheres, it is certain that the gas it contains will reach a supersonic regime when discharging in the atmosphere. This is well confirmed by the complex shock wave pattern (shock diamonds) very specific to supersonic flows and first described by Mach,¹⁰ which is clearly visible in our CFD simulations (Fig. 1 (500 μ s) and Fig. 2 (518 μ s)).

The CFD simulations reveal that the cork popping is followed by successive flowing phases, the reader must refer to the simulations rows shown in Fig. 1 corresponding to 500, 917 and 1167 μs , respectively, as well as to the evolution of the Mach number of the gas versus time presented in Fig. 2 from 166 to 1577 μs .

During the early phase closely following the cork ejection (for example for a flowing time of 500 μs as shown in Fig. 1; see also Fig. 2 (166, 249, 415 and 518 μs)), the cork is so close to the throat of the bottleneck that the pressure of the gas located between the cork and the bottle is still several bars, much higher than the critical pressure. The flow comprised in the small volume between the bottleneck and the cork stopper is not choked along the bottle axis and remains subsonic. The gas is accelerated until it reaches a maximum speed of about 200 m.s^{-1} at the bottleneck. This speed corresponds to a Mach number of 0.78 (Fig. 3) which indicates that the speed of sound has not yet been reached at the bottleneck. This results in deceleration of the gas after the bottleneck to zero speed at the cork. Interestingly, the temperature of the gas at the bottleneck drops to -43°C before rising to -10°C at the cork, thus explaining the formation of water ice observed on the internal face of the cork during this initial phase of ejection.⁶ The high pressure gas in the region under the cork has no alternative but to escape laterally into atmospheric air giving rise to a nice crown shaped supersonic expansion characterized by a typical succession of shock cells along which the expanding gas gradually equilibrates its static pressure to ambient pressure. Although the lateral diamond shocks were not revealed by the high speed camera,^{5,6} their presence seems to be confirmed by another unpublished numerical simulation.²² From Fig. 2, it can be seen that the Mach number of the supersonic jet crown reaches about 2.9 in the very early stage of the lateral gas expansion ($< 249 \mu\text{s}$).

A second phase begins once the cork is far enough from the bottleneck so that the pressure downstream is lower than the critical pressure. In that case, the bottleneck can behave as a sonic throat and the gas flow is accelerated downstream to reach supersonic speed up to Mach 1.6-1.8 (see second row of Fig. 1, relative to 917 μs ; see also panels 747, 913 and 996 μs of Fig. 2). The enthalpy of the gas is converted into kinetic energy leading to a drop in temperature down to -95°C then triggering the condensation of CO_2 , as observed in our previous work.⁶ The fluid molecules then impinge on the cork face and rebound leading to the formation of a bow shock which can be seen as the coalescence of reflected signals by the object. The shock is a compression front across which the flow properties jump. According to the second law of thermodynamics, a flow behind a normal shock wave is necessarily subsonic²¹. The distance between the bow shock and the object, i.e. the thickness of the shock layer, depends on the Mach number and cannot be determined using a simple analytical expression, it needs to be determined by numerical calculation methods as the one used in the present work.

As confirmed by our simulations, the flow behind the shock wave is subsonic, its temperature is raised to $\sim -60^\circ\text{C}$ and the gas is recompressed to about 2.2 bar so that it further expands laterally up to recover a supersonic regime responsible for the formation of lateral shock cells. The simulations clearly show that the radial ejection of the gas during the initial phase (phase 1) is followed by a purely axial ejection once

the normal shock wave is formed at the bottle outlet (phase 2). Gas escapes laterally only after passing through the shock wave and impacting on the plug.

During the third phase the pressure of the gas in the bottle has become too low to maintain a $NPR > 2$, the choked conditions are not anymore satisfied, neither at the bottleneck nor at the edge of cork. The normal shock wave and the crown shaped lateral shock cells can no longer form (see last row in Fig. 1 corresponding to a time flow of 1167 μs ; see also Fig. 2 for times greater than 996 μs). The flow is now subsonic and a rarefaction wave propagates in the bottleneck.

Position of the detached shock. Figure 4 shows the evolution of the calculated position of the bow shock as a function of the pressure in the bottle (the open symbols correspond to the position of the rarefaction wave which propagates inside the bottleneck). The position of the bow shock is compared to the position of the Mach disk that would ideally form if the jet did not hit the cork, which is of course only an abstraction. The position of the Mach disk is calculated from the study of Orescanin *et al.*¹⁸ on free jets issued from finite reservoirs. This X_{Mach} position depends on the ratio between the high pressure of the reservoir (p_0) and the external pressure (p_{ext}), for pressure ratios less than 15 it is given by the relation

$$\frac{X_{Mach}}{D} = 0.41 \left(\frac{P_0}{P_{ext}} \right)^{0.66}, \text{ where } D \text{ is the diameter of bottle outlet. The Mach disk gets closer as gas}$$

escapes and cylinder pressure drops. However, it remains much further from the opening of the bottle than the bow shock, which shows that it is the cork that controls the formation of the shock waves.

The normal shock wave could be observed experimentally (Fig. 5) due to the light scattered by the solid CO_2 particles which formation is triggered by the very low temperature reached by the flow during its adiabatic cooling.^{5,6} The calculated distance of the shock wave from the cork is generally in good agreement with the observations, with nevertheless a better agreement for longer flowing times (Fig. 6). These small disagreements could be explained by the presence of condensation of water and CO_2 molecules which is not taken into account in our CFD simulations although responsible for an important release of heat of condensation in the flow. Not surprisingly, the shock detachment distance reduces when the Mach number increases, i.e. with increasing bottle pressure. Although difficult to model and predict, it is a well-known effect observed in many studies of gas dynamics.^{19,23} Additional simulations were performed for lower initial pressure conditions of 3, 5 and 6 bar (Fig. 7). They do confirm observations: the normal shock wave is as close to the cork stopper that upstream pressure is strong.

Discussion

Our CFD simulations reveal the existence of three distinct flowing phases following the cork popping of a bottle of champagne. In the early phase, between 0 and 600 μs approximately (time 0 corresponding to the precise moment when the cork stopper separates from the bottleneck), the gas which leaves the bottle is axially blocked by the cork. The situation is then very different from a gas which would escape freely from a high-pressure reservoir into the atmosphere. In the case of an unobstructed free stream

downstream, the gas outlet would behave like a sonic throat, causing the gas to accelerate beyond the speed of sound. In the presence of the stopper and during this initial phase, the gas which escapes from the bottle does not have the possibility of expanding sufficiently along the axis of the cylinder, so that the Mach number at the bottleneck remains less than 1. The bottleneck therefore does not behave like a sonic throat: the gas reaches its maximum (subsonic) speed at the bottleneck after its acceleration under the effect of the progressive narrowing of the outlet section of the bottle, then decelerates downstream of the bottleneck under the effect of the sudden increase in the outlet section. In this first phase of the process, the gas located between the cork stopper and the bottle outlet is characterized by a pressure of several bars and it will obviously seek to balance its static pressure with atmospheric pressure by escaping laterally through the annular space which grows as the cork is ejected. Numerical simulations show that this space acts actually as an annular sonic throat. The gas escapes radially at supersonic speed, balancing its pressure through a succession of right and oblique shock waves forming the usual structure of diamond shock waves clearly visible in the simulations (see Figs. 1 and 2), note that the axial symmetry of the bottle leads to a crown-shaped supersonic expansion.

In a second phase, typically between 600 and 1000 μs , the gas pressure at the bottle outlet has become low enough for the critical condition (Mach 1) to be reached at the bottleneck (see e.g. Fig. 3). Then gas escapes from the bottle at supersonic speed, this time directed along the axis of the cylinder. The gas then impacts the cork stopper and becomes subsonic again passing through a detached shock (bow shock) induced by the presence of the cork stopper. The position of this bow shock wave agrees well with the observations. It must be underlined that this shock wave corresponds to a bow shock rather than the characteristic Mach disk of non-adapted free jets that would form further away in the absence of a cork stopper.

Finally, in the last phase, typically beyond 1000 μs , the pressure in the bottle is too low to maintain the critical pressure at the bottleneck. The gas leaves the bottle at subsonic speeds and then decelerates downstream. The simulations clearly show the propagation of a rarefaction wave inside the bottle during this last phase.

Methods

Computational domain and initial conditions. The axisymmetric geometry approximation is chosen because it is well suited to the axial symmetry of the flow field corresponding to the gas ejection during champagne cork popping from a bottle held vertically. One of the calculation domains (Fig. 8) concerns the internal gaseous volume of approximately 35 cm³, under pressure, found within the bottleneck of the champagne sealed bottle (i.e., the gas phase between the liquid surface and the cork stopper). This gas mixture consists in gas-phase CO₂, with traces of water vapor, nitrogen, ethanol vapor and a myriad of other volatile compounds.¹ Nevertheless, the partial pressure of gas-phase CO₂ is largely dominant compared with that of all other gaseous compounds.¹ For the sake of simplicity, the numerical simulations were therefore carried out by considering that the gas phase under pressure in the bottleneck

of the corked bottle consisted in pure CO₂. Moreover, the initial pressure and temperature were respectively set at 7.5 bar and 20°C, in order to comply with one of the experimental conditions imposed in previous studies.^{5,6} The calculations are based on the exact geometric profile of a bottle of champagne. In the headspace, the section of the bottleneck gradually reduces until it reaches an internal diameter close to 1.8 cm at the outlet of the bottle. The other part of the calculation field concerns the external environment formed by the ambient air in which the CO₂ will expand freely.

The movement of the champagne cork is controlled with a user-defined function (UDF) imported from the ANSYS Fluent software. This function fixes the ejection speed of the cork stopper at 18.6 m.s⁻¹ established from experimental observations made under the same flowing conditions⁵ (Fig. 9). Note that for the sake of simplicity, in our simulations the elasticity of the cork has not been taken into account, which explains why in our simulations the base of the cork does not adopt the typical mushroom shape of a champagne popped cork (see inserted picture in Fig. 4) but remains cylindrical once removed from the bottle (Figs. 1 and 2).

Calculation method. Our fluid dynamics calculation study is based on the commercial ANSYS Fluent software. More specifically, in the present study, Navier-Stokes axisymmetric equations and species transport equations are used, and all flow variables are used in the mixing forms. The k-epsilon turbulence model (“Realizable” option) is used, and the Near-Wall Treatment (“Enhanced Wall Treatment” option) is selected. The “pressure-velocity coupling” algorithm is chosen for the calculation process. The “PRESTO” model is used for the discretization of the pressure and to obtain a good precision of the pressure gradients near the walls. The “Second Order Upwind” model is selected for the discretization of momentum and energy equations. Considering the cork stopper velocity and the Courant-Friedrichs-Lewy (CFL) condition, the computational time interval is set to 10⁻⁶ s, and the maximum number of iterations for each time step is set to 200. The external limits of the domain of integration were maintained at ambient temperature and pressure.

Dynamic mesh. The calculation domain is modified as the cork stopper is ejected. It is therefore necessary to use a dynamic mesh to simulate the gas flow throughout the ejection of the cork stopper. Smoothing and remeshing methods are used and properly parameterized to maintain a high mesh quality and avoid any degeneration of the grid during its updating and deformation throughout the calculation process. The diffusion-based smoothing method is used for the mesh deformation with a limit distance and a diffusion parameter set to 0.1. The local remeshing method is used when the mesh violates the skewness or size criteria²⁴. The minimum and maximum length scales parameters are set to 10⁻⁶ m and 0.002 m, respectively, and the maximum cell skewness is fixed to 0.7.

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Figures

Figure 1

Simulation of pure CO₂ expanding freely into ambient air (20°C, 1.013 bar) following the cork popping of a champagne bottle initially kept at 20 °C with an inner pressure of 7.5 bar. The first, second and third panel rows relate respectively to flowing times of 500, 917 and 1167 ms measured after the cork popping. The first, second and third panel columns are relative to the flow velocity, static pressure and temperature, respectively.

Figure 2

Simulation of the Mach number versus time of pure CO₂ expanding freely into ambient air following cork popping. The bottle is initially kept at 20 °C and 7.5 bar. The first seven images of the series reveal the supersonic character of the flow (Mach > 1) whereas it is subsonic (Mach < 1) from the eighth image because the pressure in the bottle has become subcritical.

Figure 3

Mach number axial profile of a gas escaping from a bottle initially at 20°C and 7.5 bar for flowing times of 500, 917 and 1167 ms. At 500 μ s (phase 1) the exit pressure is too high so that the gas flow is not choked along the bottle axis, it decelerates downstream the bottleneck. At 917 μ s (phase 2), the flow is supersonic and a detached shock is forming in front of the cork. At 1167 μ s (phase 3), the pressure in the bottle is too low and nozzle pressure ratio (NPR) is not high enough for maintaining a choked flow on the bottle axis.

Figure 4

Comparative position of the Mach disk and the bow shock. Blue dots: position of the Mach disk which would form in the absence of a cork during the discharge of gas into the atmosphere. Red dots (full symbols): simulated position of the bow shock. Red dots (open symbols): simulated position of the rarefaction wave.

Figure 5

Calculated and observed positions of the normal shock wave. Here, the bottle was initially kept at 20°C and 7.5 bar, both simulation and picture corresponds to a flowing time of 917 μ s after the cork popping. The origin of the x-axis corresponds to the surface of the liquid in the bottle.

Figure 6

Temporal evolution of the calculated and observed positions of the detached shock wave forming in front of the cork.

Figure 7

Calculated positions of the detached shock wave for different initial bottle pressures ranging from 3.0 to 7.5 bar. In the present simulations, the pressure in the bottle was kept constant and the distance between the outlet of the bottle and the cork was kept at a fixed position. The higher the Mach number, the closer the shock forms to the cork.

Figure 8

Mesh of the computational domain at initial time.

Figure 9

Position of the cork stopper as a function of time. The position results from experimental observations from which an ejection speed of 18.6 m.s^{-1} is obtained for a champagne bottle initially kept at 20°C with an inner pressure of 7.5 bar.