Bubbles In, Air Out: Realistic Simulation Helps Keep the 'Pop' in Soft Drinks

Coca-Cola design engineers use Abaqus to analyze carbon dioxide and oxygen flow in plastic beverage bottles

An ice-cold soft drink is one of life's reliable pleasures on a hot day. The whoosh of sound when you twist off the cap of the bottle, the icy tingle of bubbles on your tongue, the crisp taste as you swallow the refreshing liquid. But occasionally this simple joy falls flat: When you twist off the top there's no fizz. When you take your first gulp the drink is dull and tasteless. What exactly has gone wrong?

Engineers who design beverage bottles for Coca-Cola know precisely what has happened because it's their job to ensure that customers don't experience fizz-flop or tepid-taste in any of their soft drinks. After all, as the world's largest beverage company with more than 500 sparkling and still brands, Coca-Cola provides about 1.8 billion drinks daily in more than 200 countries.

Their research and development teams are charged with maintaining the optimum levels of carbon dioxide (CO_2) *inside* bottles to preserve fizz (in those drinks that are supposed to bubble). They also work to keep *out* oxygen (O_2) as long as possible, to avoid compromising taste and freshness in both carbonated and still liquids (such as fruit juice, milk, and tea). And Coca-Cola's distributors around the globe count on such expertise to guide them about storage temperatures and expiration dates.

Advantages of plastic bottles come with new challenges to designers

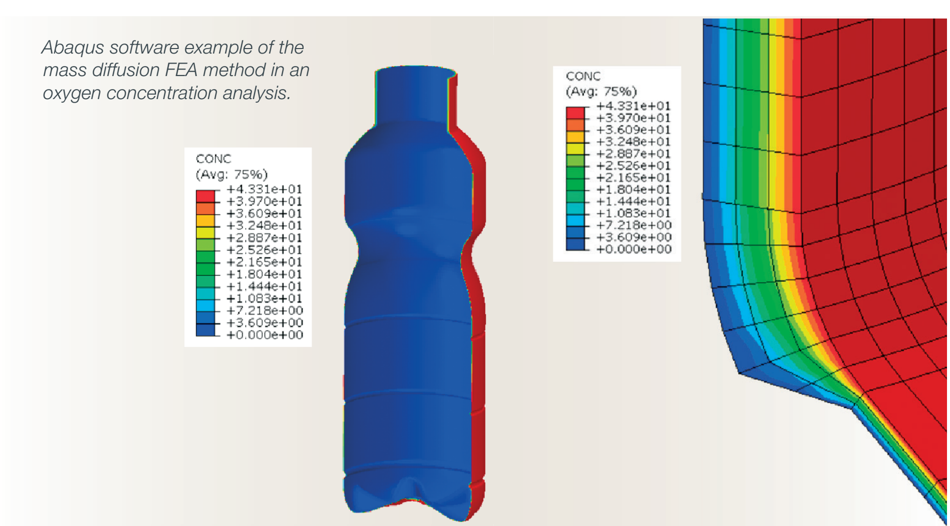
Back when soft drinks were freshly made at pharmacy soda fountains or carried home in capped glass bottles, fizz and taste could be pretty much guaranteed. Then soda fountains gave way to vending machines, aluminum cans replaced heavy glass, and finally plastic bottles came on the scene. Lighter, less-expensive, resealable, recyclable plastics provide many advantages to both consumers and bottlers. Yet maintaining product uniformity in the face of time, climate, and travel has become more of a challenge.

The widely used polyethylene terephthalate (PET) beverage bottle of today is made from one of the more impervious of plastics—40 times more efficient than high-density polyethylene (HDPE), for example—but CO_2 and O_2 nevertheless trickle slowly through its walls over time. PET bottles are manufactured via a melting-and-forming, 'stretch-blow molding' process that orients and crystallizes the plastic on the molecular level. This affects the movement of the two gases through the bottle walls in distinct, complex ways. Although you can see the amount of CO_2 bubbles in a drink for a rough gauge of its fizziness, human eyes are certainly not precise measuring instruments. And taste-robbing oxygenation with O_2 is a largely invisible process. What's an engineer to do?

Finding virtual answers to real-world questions

Realistic simulation—the 3D computer representation of an object, the forces that can impact that object, and the resulting stresses and strains over time—has provided Coca-Cola's engineers with important answers. Their Virtual Packaging Development System is based on Abaqus finite element analysis (FEA).

Using FEA, Coca-Cola engineers have developed a 'virtual bottle model' that they can modify on their computer screens into whatever shape or material they want, depending on the type of beverage it will be



Abaqus software example of the mass diffusion FEA method in an oxygen concentration analysis.

filled with and the manufacturing process that will be used to make it. They can then simulate the effects on the bottle of stacking, crushing, dropping, and sloshing to prove out their designs, quickly and cost-effectively modifying the shapes to make bottles lighter, thinner, stronger, and so on. Having validated their computer models with real-world tests, they now have a 'library' of highly reliable simulations they can use to perfect existing designs and shorten time-to-market for new ones as products, consumer preferences, and industry regulations change.

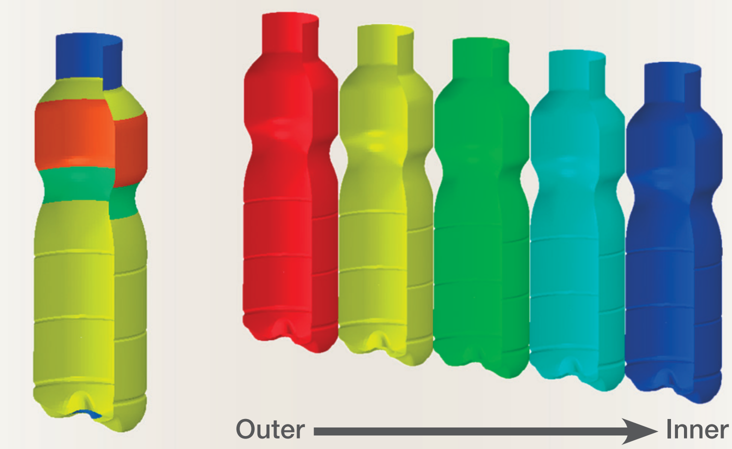
How do you simulate what's invisible?

For a design engineer, it's fairly straightforward to use FEA to simulate a plastic soft drink bottle hitting the floor. But what about predicting how tiny, invisible molecules of CO_2 or O_2 gas migrate through the walls of that bottle? The engineers at Coca-Cola Beverage Co. Ltd's Global Innovation & Technology Centre (GITC) in Shanghai decided to try. And thanks to the unchanging laws of physics, and some pretty cool capabilities in their software tools, they've succeeded.

The team started with the oxygen problem. How much O_2 passes into a beverage bottle through its PET wall per day? A simulation of this O_2 transmission rate (OTR) phenomenon needed to consider the effects of the bottle's geometry, the 'thickness profile' of the PET wall (thicker or thinner in different places depending on the manufacturing process and the curves of the bottle), and the material characteristics of each 'zone' of bottle thickness (where crystallinity, diffusivity, and solubility can vary).

"We investigated two different ways to tackle this problem with Abaqus software," says Dr. Simon Shi, senior packaging engineer at GITC. His team first applied the mass diffusion procedure, which simulates the movement of a fluid through a solid over time. Employed in such diverse industries as electronics and energy, it can be applied to everything from moisture absorption in the electronics chip of a phone to hydrogen embrittlement (gas migration through metals) inside a nuclear reactor. In the case of a PET bottle simulation, the 'fluid' moving through the solid is the oxygen.

The mass diffusion procedure starts with an FEA model of the bottle that incorporates the material properties of PET and the as-manufactured wall thickness profile,



The heat transfer method is an alternative analysis available in Abaqus.

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previously determined from physical tests. A pressure gradient is loaded into the model to set the starting oxygen concentration inside (lower) and outside (higher) the bottle. When the diffusion simulation is run, the flow of oxygen passing through the bottle wall (always from higher to lower concentrations) appears on the computer screen as a moving rainbow of changing colors (blue is lower, red is higher). The flow will be higher across the thinnest areas of the bottle where there is less plastic for the oxygen to get through, and it will also be affected by the material properties, particularly the cystallinity. "The mass of O_2 that builds up on the inside wall of the bottle over time is what diffuses into the liquid to affect taste and freshness," says Dr. Shi.

Another FEA technique the engineers considered was Abaqus' heat transfer method. This is commonly used in the automotive industry to study thermal performance of powertrain assemblies, and in the electronics industry to analyze heat and power cycling of components. "The governing equations used to solve the O_2 question are the same for heat transfer as for mass diffusion," says Dr. Shi, "but in this case we were looking at the conduction of temperature (instead of the change in concentration of gas) from one side of the bottle to the other."

With the heat transfer method, the team could use a different type of 3D element as the building block for their models. Elements, used by the hundreds of thousands in an FEA model, are the mathematical units that describe the object being analyzed. "We found that the 'shell' elements available in the heat transfer method were more efficient," says Dr. Shi. "They use less computational time than the solid 'hex' ones used in the mass diffusion procedure and gave us slightly more accuracy in this particular case." As they ran their models, the engineers monitored the heat flux on the inner surface of the bottle, which varies over time due to PET wall thickness and material properties.

The engineers did some post-processing of their results from the heat and the mass simulations and found that predicted O_2 flow rates from both methods came very close to real-world measurements of about 0.04 milliliters of oxygen passing from outside to inside a bottle per day. "This doesn't sound like much on a daily basis," says Dr. Shi, "but if that bottle sits on the shelf for too long, those milliliter fractions of oxygen will mount up and impact beverage quality." In a bottle of juice, for example, each 1 mg of O_2 that gets into the solution can consume 11 mg of Vitamin C, depleting the nutritional value of the drink

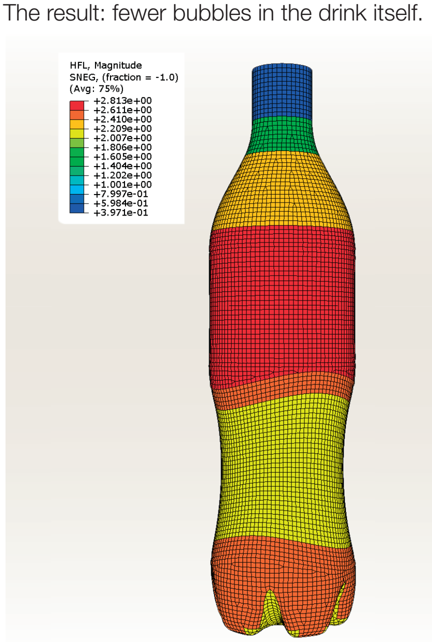
Continued

over time. Knowing now what the oxygen rise rate is—and how to simulate it in their virtual bottle models—Coca-Cola engineers can optimize PET bottle shape, wall thickness, and manufacturing processes to minimize it.

That bottle sitting on the shelf is actually moving

The second challenge, simulating CO_2 loss, required more steps to solve since the physics of pressure change are more complex than those of oxygen concentration. Freshly bottled Coca-Cola has an inside CO_2 pressure of 60 psi (about the same inflation as a compact spare tire). This provides that satisfying whoosh sound when opened as well as those tingles on the tongue and down your throat as you drink. When the pressure drops to 78.6% of the initial value the liquid goes "flat." The question is, how long does it take for the drop to occur, and therefore, what is the shelf-life of the product?

To complicate the picture, pressure loss is not due solely to CO_2 leaking out as oxygen leaks in. The bottle itself is also expanding slightly, or 'creeping,' over time due to the internal pressure. While creep is a natural characteristic of many materials, in a plastic soda bottle it causes the total volume inside the bottle to gradually get bigger, resulting in a secondary drop in pressure. Lower pressure inside the bottle allows more CO_2 to escape from the beverage into the empty space between liquid and cap. The result: fewer bubbles in the drink itself.



An example of a CO_2 loss rate analysis in Abaqus. A greater proportion of the gas passes through the thinner areas of the bottle.

To make their simulations of creep as realistic as possible, the engineers began with a laboratory test of a bottle containing some dry ice (frozen CO_2), which would evaporate to create the target pressure of 60 psi. Then they measured how much the bottle dimensions crept over one week, while at the same time tracking the CO_2 loss rate. "Starting from these real-world tests gave us highly accurate values for crept-bottle shape, volume, and pressure that we could build into our virtual bottle model," says Dr. Shi.

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Now the team was ready to run a heat-transfer method CO_2 analysis on their virtual bottle, similar to what was done with the oxygen simulations. Of course this time the pressure gradient was set up in reverse from the oxygen flow model, with higher levels set inside instead of outside, to reflect the CO_2-charged state of the bottle. Plugging the crept-bottle measurements into their model, the engineers could then run their analyses to predict both pressure and volume changes over time.

"Simulating these processes takes about two hours—much less time than with physical measurements recorded over a week in the laboratory," says Dr. Shi. "And O_2 flow simulations only take a couple of minutes. Our FEA models now predict the flow of both carbon dioxide and oxygen gases in PET bottles very reliably. This gives us a more complete picture of what will happen to our products in the real world and provides an efficient way to evaluate bottle performance at the early stages of design."

Proving out new concepts and delivering beverage quality

The Coca-Cola engineers see continuing value in their new methodologies going forward. "Bottles are getting lighter and thinner in response to economic and environmental realities," says Dr. Shi. "We now have a validated methodology in Abaqus that we can use to prove out new concepts in shape and material thickness.

"We plan to explore the behavior of other materials besides PET, such as plant-based plastics, in the future. Realistic simulation gives us confidence that we will always be able to cost-effectively provide product quality to our customers anywhere in the world market."

The history of 'soda pop'

The inspiration for 'soda pop' can be traced back to ancient times, when people thought bathing in naturally carbonated mineral springs could promote health and cure diseases. If dipping in such water was good for you, then shouldn't drinking it be even better?

That's what Joseph Priestley was thinking when he created the first man-made, drinkable glass of carbonated water in 1767. Experimenting with gases in his local brewery, he discovered that distilled water suspended over a fermentation vat became infused with carbon dioxide, taking on a tangy, bubbly taste. Others learned how to directly add CO_2 to water, as either dry ice or a high-pressure liquid, and then began mass manufacturing the increasingly popular beverage.

Flavored syrups were refined by chemists in the late 19th century, and the soda fountain blossomed as a community center where people went to socialize and enjoy a fizzy beverage. Some pharmacists' syrup formulas (like Coca-Cola's secret one) developed into brands still known today. The advent of bottling factories made soft drinks portable and storable and by 1920 over five thousand bottling companies were registered with the U.S. Census Bureau. Consolidation means that fewer major brands survive today—but soft drinks remain as popular as ever all over the world.