Simplified approaches for modelling a sealed and partly fluid filled container

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Abstract: Containers (bottles) made of polymers are exposed to manifold loads during their life cycle. They are open or sealed as well as empty or filled. Depending on the mentioned conditions a container behaves different under loading. This effect can be observed in everyday life. Imagine opening a shaken plastic bottle filled with a carbonated beverage. Abaqus provides simulation methods for completely filled containers with either a pneumatic or a hydraulic fluid. Real containers barely are totally filled with a hydraulic fluid. In general there is always a so called head space filled with gas (pneumatic fluid). This paper presents two methods for modelling the two-phase system (liquid and gas) inside a partly filled container using a fluid cavity instead of meshing the volume inside the container. Therefore a one-phase system equivalent to the two-phase system is described and applied to the model using two different methods – an explicit and an implicit one. These methods are implemented by using subroutines which allow extending the functionality of Abaqus. Applying these approaches allows cost efficient simulations of various loads like excess pressure, vacuum, temperature change, top load, squeezing etc. for sealed, partly filled containers. The paper describes the background and assumptions necessary to define the one-phase system, verifies the model by comparing the FEA results with analytical solutions and shows worked examples.

Keywords: Container, Bottle, Partly Filled Container, Consumer Packaged Goods, Hot Fill, Fluid-Structure Interaction, Fluid Cavity, Multi-Phase Simulation, Ideal Gas and Bulk Modulus.

1. Introduction

To accelerate and improve the development of new containers (bottles) made of polymers the use of numerical simulations nowadays is state of the art. As short as the lifetime of containers for consumer packaged goods (CPG) seems to be, as manifold are the conditions and loads they are exposed to. Each condition and loading type requires different simulation techniques to ensure efficient development. Typically process simulations of extrusion blow moulding process (EBM) or stretch blow moulding process (SBM) are performed to predict the wall thickness distribution off a container. Product simulations predict the behaviour of the bottle exposed to different loads and different conditions. Some product simulations correspond directly with tests usually performed during customer approval procedure or for quality assurance. Classically these are:

- Top load test / simulation
- Squeezing test / simulation
- Bulging test / simulation

Figure 1 shows a typical top load test configuration where a bottle is located between a bearing plate on the bottom and a bearing plate on the top. The top plate is moved downward and the load-displacement curve is recorded.

Figure 1. Top load test (left), simulation (right).

Other product simulations are not related to physical tests or are replacing expensive and time consuming tests. A question of interest for such a simulation can be the behaviour of containers filled with hot liquid and sealed at high altitude, afterwards while cooling they are transported to see level where they are palletized. Simulations of this kind are required in order to ensure a proper performance of the container during its entire life cycle. Looking at a containers life cycle there are phases during which the container is either open or sealed. In both cases the container is empty or filled with liquid. Even in a filled container there is always a so called head space containing gas. Figure 2 illustrates these four possible conditions.

Simulations dealing with condition (a) in Figure 2 just have to consider the mechanical properties of the material the container is made of. In case of condition (b) for many simulations fluid sloshing and gravity effects of the fluid mass can be neglected and the fluid can be modelled by applying hydrostatic pressure on the bottle. Condition (c) can be well modelled in Abaqus/Standard and Abaqus/Explicit using surface-based fluid cavity technique. It provides the coupling between the deformation of the fluid filled structure and the pressure exerted by the contained fluid on the cavity boundary of the structure (Dassault Systémes Simulia Corp., 2014). This technique supports two different types of fluids:

- Pneumatic fluids
- Hydraulic fluids

Pneumatic fluid can be used to model condition (c) in Figure 2.

Condition (d) in Figure 2 is characterized by the presence of two different fluids – a pneumatic fluid (gas) and a hydraulic one (liquid).

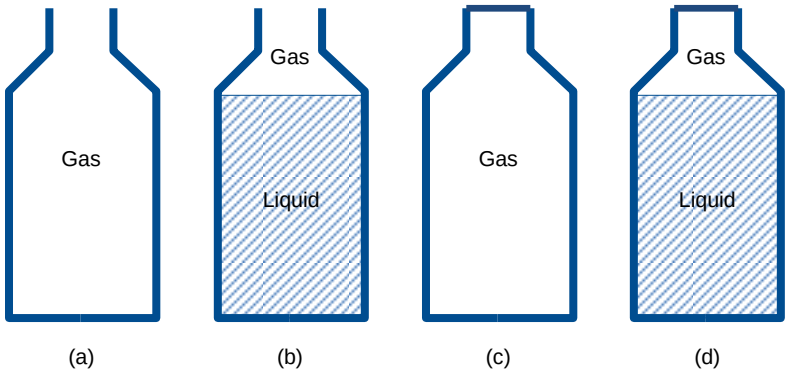

**Figure 2. Conditions of a container during its life cycle –
(a) empty/open, (b) partly filled/open, (c) empty/sealed, (d) partly filled/sealed.**

For cases where fluid sloshing and gravity effects of the fluid can be neglected a surface-based fluid cavity filled with a single artificial bulk (see Figure 3) can be used to model this condition. In the following two approaches achieving this goal are presented.

2. Modelling approaches for partly filled/sealed containers

In order to avoid expensive meshing of the volume inside the container and describing liquid and gas by constitutive models an approach using surface-based fluid cavity is chosen.

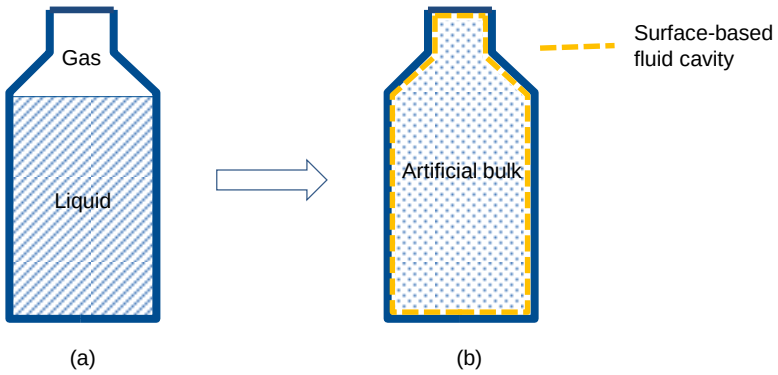

**Figure 3. Partly filled/sealed container –
(a) two-phase system and (b) equivalent one-phase system.**

To describe the properties of the artificial bulk inside the fluid cavity two different approaches are presented.

The first approach is an implicit one using the user subroutine UFLUID of Abaqus/Standard to define the constitutive model of the artificial bulk.

The second approach – an explicit one – can be applied to Abaqus/Standard as well as to Abaqus/Explicit. Therefore the artificial bulk is considered as hydraulic fluid but with a fluid cavity pressure (gauge pressure) dependent bulk modulus $K(p)$.

2.1 Implicit approach using subroutine UFLUID

User subroutine UFLUID serves to define a fluid constitutive model being used for hydrostatic fluid elements used in cavities. The subroutine requires the definition of the fluid density $\rho(p,\theta)$, where p is the fluid cavity pressure and θ is the fluid cavity temperature, its fluid pressure compliance

$$C_p = -\rho^{-2}\frac{d\rho}{dp} \tag{1}$$

and the fluid temperature compliance C_θ defined as (Dassault Systémes Simulia Corp., 2014):

$$C_\theta = -\rho^{-2}\frac{d\rho}{d\theta} \tag{2}$$

2.1.1 Fluid density $\rho(p,\theta)$

Let's consider a container as shown in Figure 4 (a) exposed to an ambient pressure p_{amb}. Inside the container an initial fluid cavity pressure (initial gauge pressure) p_{ini} is acting. The gas with the initial volume $V_{G,ini}$ and initial temperature θ_{ini} is considered to be an ideal gas with the specific gas constant R_s. The absolute initial pressure $\tilde{p}_{ini}$ results from the ambient pressure p_{amb} and the gauge pressure p_{ini} to:

$$\tilde{p}_{ini} = p_{amb} + p_{ini} > 0 \tag{3}$$

According to the equation of state (EOS) of an ideal gas its density is (Cerbe & Wilhelms, 2005)

$$\rho_{G,ini} = \frac{\tilde{p}_{ini}}{\theta_{ini} * R_s}. \tag{4}$$

The gas mass m_G inside the container remains constant and can be calculated as follows:

$$m_G = m_{G,ini} = \rho_{G,ini} * V_{G,ini} \tag{5}$$

The liquid is considered to be incompressible and the volume V_L independent of the temperature. Hence its density ρ_L and mass m_G is constant:

$$m_L = \rho_L * V_L = const. \tag{6}$$

The total container volume V_{ini} of the initial configuration (a) in Figure 4 is the sum of the initial gas volume $V_{G,ini}$ and the constant liquid volume V_L. In addition the initial fraction of liquid $L_{frac,ini}$ in the cavity is defined by:

$$L_{frac,ini} = \frac{V_L}{V_{ini}} = \frac{V_L}{V_{G,ini} + V_L} \tag{7}$$

Looking at the deformed configuration (b) in Figure 4 the state of the gas is described by the fluid cavity pressure p leading to the absolute pressure

$$\tilde{p} = p_{amb} + p > 0, \tag{8}$$

the temperature θ and the volume

$$V_G = \frac{\tilde{p}_{ini} * V_{G,ini} * \theta}{\theta_{ini} * \tilde{p}} \tag{9}$$

which results from the EOS of an ideal gas. The process leading from the initial configuration to the deformed one is considered to be isotherm.

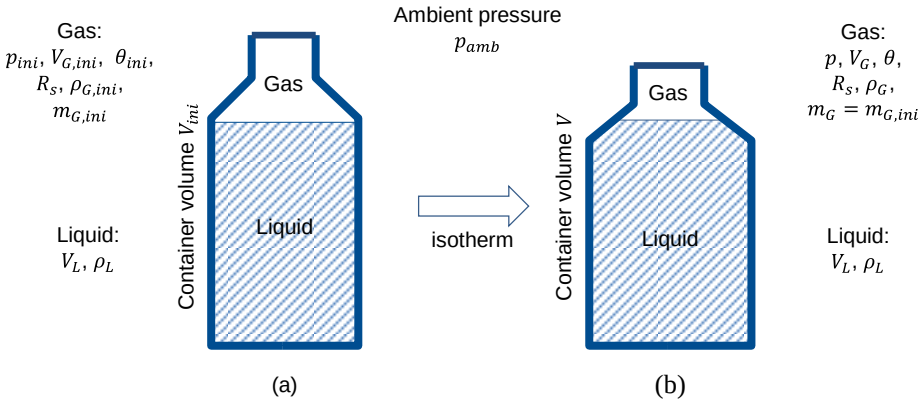

Figure 4. Partly filled/sealed container –
(a) initial configuration and (b) deformed configuration.

The total mass m inside the deformed configuration (b) in Figure 4 is calculated from the mass of the gas m_G and the mass of the liquid m_L. Taking equations (5) and (6) leads to:

$$m = \rho_{G,ini} * V_{G,ini} + \rho_L * V_L \tag{10}$$

The total volume V is the sum of the gas volume V_G and the constant liquid volume V_L. Considering equation (9) leads to:

$$V = \frac{\tilde{p}_{ini} * V_{G,ini} * \theta}{\theta_{ini} * \tilde{p}} + V_L \tag{11}$$

Since the density $\rho(p, \theta)$ of the deformed configuration (b) in Figure 4 is required one now can take equations (10) and (11) to obtain:

$$\rho(\tilde{p}, \theta) = \frac{m}{V} = \frac{(\rho_{G,ini} * V_{G,ini} + \rho_L * V_L) * \theta_{ini} * \tilde{p}}{\tilde{p}_{ini} * V_{G,ini} * \theta + V_L * \theta_{ini} * \tilde{p}} \tag{12}$$

Taking advantage of equation (8) and of $L_{frac,ini}$ defined in equation (7) reforming equation (12) leads to the following expression:

$$\rho(p, \theta) = \frac{(\rho_{G,ini} * (1 - L_{frac,ini}) + \rho_L * L_{frac,ini}) * \theta_{ini} * (p_{amb} + p)}{\tilde{p}_{ini} * (1 - L_{frac,ini}) * \theta + L_{frac,ini} * \theta_{ini} * (p_{amb} + p)} \tag{13}$$

Equation (13) is the required expression for the density of the artificial bulk (see Figure 3) to be used in the user subroutine UFLUID.

2.1.2 Fluid pressure compliance C_p and fluid temperature compliance C_θ

As described in section 2.1 the user subroutine UFLUID requires the definition of the fluid pressure compliance C_p and the fluid temperature compliance C_θ as defined in equations (1) and (2). Applying equation (13) to the definition of C_p and C_θ one obtains following two expressions needed for the user subroutine UFLUID:

$$C_p = -\frac{\tilde{p}_{ini} * (1 - L_{frac,ini}) * \theta}{(\rho_{G,ini} * (1 - L_{frac,ini}) + \rho_L * L_{frac,ini}) * \theta_{ini} * (p_{amb} + p)^2} \tag{14}$$

$$C_\theta = \frac{\tilde{p}_{ini} * (1 - L_{frac,ini})}{(\rho_{G,ini} * (1 - L_{frac,ini}) + \rho_L * L_{frac,ini}) * \theta_{ini} * (p_{amb} + p)} \tag{15}$$

Equations (3), (4), (7), (13), (14) and (15) describe the constitutive model of the artificial bulk in Figure 3 consisting of the liquid and the gas phase.

2.1.3 Application of fluid properties and initial conditions to the model

Physical properties of each single phase (gas and liquid) have to be hard-coded into the user subroutine UFLUID. These are the specific gas constant R_S, the ambient pressure p_{amb}, the fluid density ρ_L and the initial liquid fraction $L_{frac,ini}$ of the initial container volume.

As Abaqus/Standard hands over the cavities reference node number to the subroutine UFLUID the node number could be used to hand over one or even more of the previous described hard-coded parameters to the subroutine UFLUID. This workaround can make the subroutine more flexible but requires attention to the node numbering of the model.

The initial fluid cavity pressure p_{ini} and the initial temperature θ_{ini} are applied to the cavities reference node.

2.1.4 Verification of the user subroutine UFLUID

In order to evaluate the accuracy of the previous described approach and the functionality of the subroutine UFLUID the simple model shown in Figure 5 is used. Therefore the fluid cavity pressure p obtained from the simulation is compared with the analytical solution.

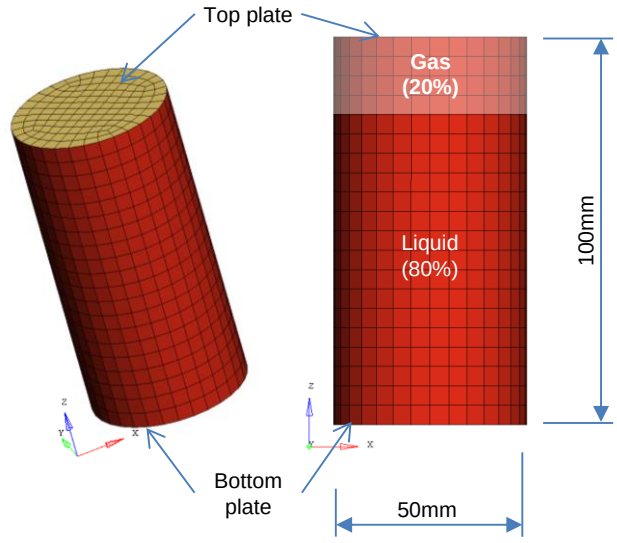

Figure 5. Rigid cylindrical tube, filled with 20% gas (air) and 80% liquid (water).

The model consists of a tube which is rigid in radial direction (achieved by constraining translational DOFs in $x-$ and $y-$direction) and sealed by rigid top- and bottom plates (achieved by constraining all DOFs). Tube and plates are modelled using S4R structural shell elements with a linear elastic material and no thermal expansion. The volume inside the tube is filled with 20% air and 80% water. I.e. the initial fraction of liquid $L_{frac,ini} = 0.80$. The following properties are used:

- Ambient pressure $p_{amb} = 0.101325$ MPa
- Specific gas constant $R_S = 288.027$ J/kgK
- Fluid density $\rho_L = 1.0e-9$ t/mm^3

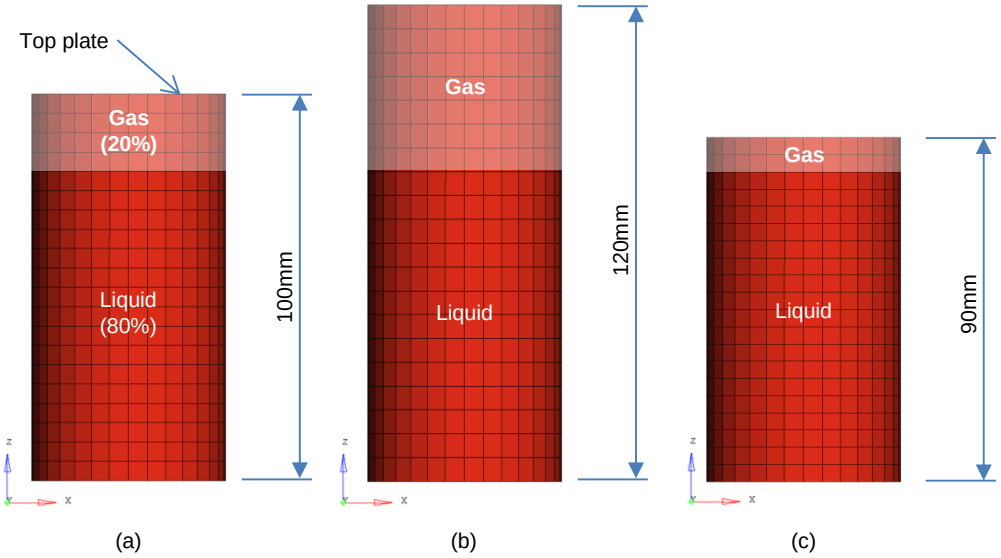

Figure 6. Cylindrical tube – (a) initial condition, (b) elongated $V_{G,ini}/V_G = 0.5$ and (c) compressed $V_{G,ini}/V_G = 2.0$.

The initial temperature is $\theta_{ini} = 350$ K. Two different values for initial gauge pressure are considered: $p_{ini} = 0.0$ MPa and $p_{ini} = 0.101325$ MPa. The inside of the tube is modelled by a surface based fluid cavity.

The following types of loads and combinations thereof are imposed to the tube:

- Change of temperature from $\theta_{ini} = 350$ K to $\theta = 280$ K
- Elongation or compression of the tube by moving the rigid top plate up- or downward (see Figure 6)

To obtain the analytical solution for the fluid cavity pressure p the gas filled head space is described by the equation of state (EOS) of an ideal gas (Cerbe & Wilhelms, 2005) and leads to

$$\frac{\tilde{p}_{ini} * V_{G,ini}}{\theta_{ini}} = \frac{(p_{amb} + p_{ini}) * V_{G,ini}}{\theta_{ini}} = \frac{\tilde{p} * V_G}{\theta}. \tag{16}$$

Considering equations (3) and equation (8) leads to the analytical expression for the fluid cavity pressure:

$$p = \frac{(p_{amb} + p_{ini}) * \theta}{\theta_{ini}} * \frac{V_{G,ini}}{V_G} - p_{amb} \tag{17}$$

Table 1 summarises the comparison between the fluid cavity pressure p calculated by simulation using subroutine UFLUID and the analytical solution according equation (17) for several load cases. Values marked with a star (*) indicate that these are the imposed loads to the model. E.g. in case 1 the fluid cavity temperature θ is decreased from the initial temperature $\theta_{ini} = 350$ K to $\theta = 280$ K while the volume of the gas is kept constant.

Table 1. Comparison of simulation and analytical solutions for gauge pressure p.

	Initial configuration	Deformed configuration			
Load case	p_{ini} [MPa]	θ [K]	$\frac{V_{G,ini}}{V_G}$ [−]	p [MPa] Simulation	p [MPa] Analytical
Case 1	0.00	280*	1.0	-0.020265	-0.020265
Case 2	0.00	280*	2.0*	0.060795	0.060795
Case 3	0.00	280*	0.5*	-0.060795	-0.060795
Case 4	0.101325	350	0.5*	0.00	-4.2e-9
Case 5	0.101325	280*	1.0	0.060795	0.060795
Case 6	0.101325	280*	2.0*	0.222915	0.222915
Case 7	0.101325	280*	0.5*	-0.020265	-0.020265

Looking to the last two columns of Table 1 it can be seen that simulations and analytical solutions are identical.

2.1.5 Application of the method to a real containers top load simulation

The modelling approach is applied to a real bottles top load simulation as shown in Figure 7. In this type of simulation the top plate is moved downward with constant velocity and the force vs. displacement curve is observed.

The bottle is discretised by means of S4R structural shell elements. Friction between top plate and bottle as well as between bottle and bottom plate is considered.

Three simulations are performed:

- **a.** Bottle empty/open
- **b.** Bottle partly filled/open with initial liquid fraction $L_{frac,ini} = 0.92$
- **c.** Bottle partly filled/sealed with initial liquid fraction $L_{frac,ini} = 0.92$

Simulations (a) and (b) don't require the described modelling approach as the bottle is open and the gas phase doesn't activate any pressure when its volume changes. The simulations (a) and (b) just serve as references for simulation (c). For all three simulations the force vs. displacement curves are plotted to be compared with each other.

The simulation (a) of the empty bottle consists of a single step during which the top plate is moved downward (in negative $z-$ direction) with constant velocity (top load simulation).

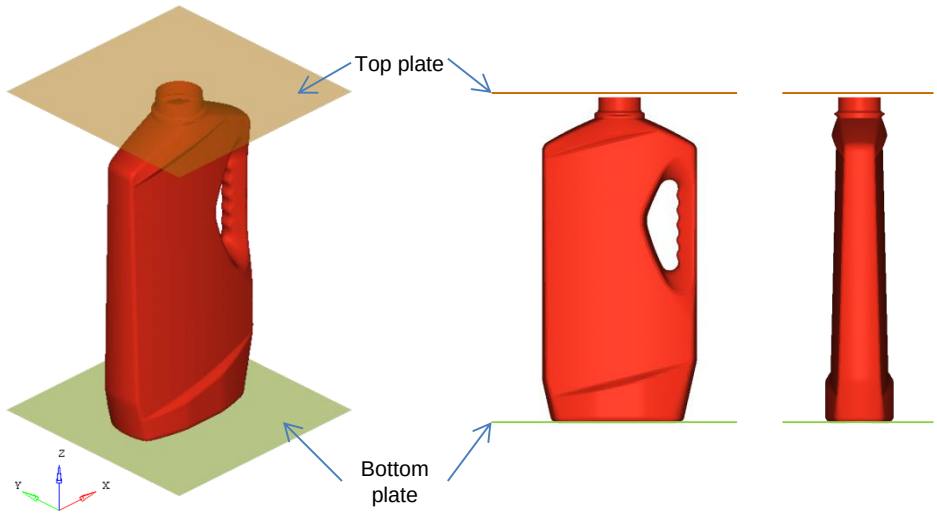

Figure 7. Model for top load simulation.

The simulations (b) and (c) of the partly filled bottle are divided into two steps (see Figure 8):

- Bulging simulation:
  The bottle is open and exposed to hydrostatic pressure leading to a deformation of the bottle (bulging). The initial liquid fraction $L_{frac,ini}$ is determined from the deformed bottle shape resulting from this step.
- Top load simulation: As described for simulation (a).

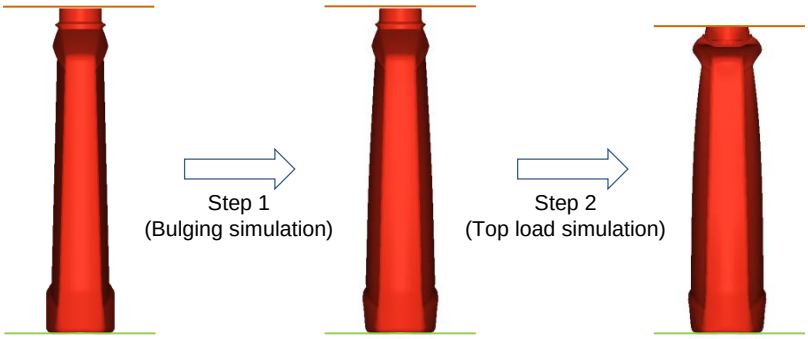

Figure 8. Partly filled/sealed bottle – not deformed (left), deformed after bulging simulation (centre) and after top load simulation (right).

Figure 9 shows the force vs. displacement curves of all three simulations.

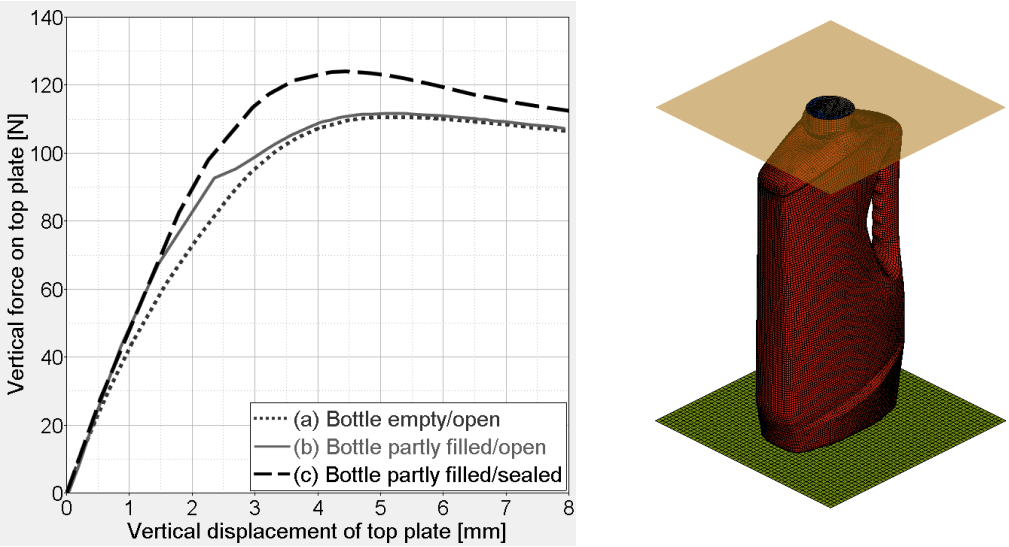

Figure 9. Force vs. displacement curves of top load simulations, deformed bottle.

The simulations (a) and (b) of the open bottle show almost the same top load peak. The partly filled/open bottle shows at the first part of the curve a little stiffer behaviour as the empty one. The partly filled/sealed bottle (c) shows an approx. 12% higher top load peak as the other simulations.

2.2 Explicit approach using pressure dependent bulk modulus $K(p)$

For surface based fluid cavities the hydraulic fluid model is used to model nearly incompressible fluid behaviour and fully incompressible fluid behaviour. Compressibility is introduced by assuming a linear pressure-volume relationship. The required parameters for compressible behaviour are the bulk modulus K and the reference density ρ_R (Dassault Systémes Simulia Corp., 2014). As shown in in Figure 3 the two-phase system should be modelled as an equivalent one-phase system. The one phase system (artificial bulk) cannot be considered as incompressible as the presence of the gas brings compressibility into the system. But with increasing compression of the gas the entire system gets stiffer. Considering a pressure dependent bulk modulus $K(p)$ instead of a constant one meets this fact.

2.2.1 Pressure dependent bulk modulus $K(p)$

A fluids bulk modulus K is described by (Dassault Systémes Simulia Corp., 2014):

$$p = -K^{*}\left(\frac{V\left(p,\theta\right)-V\left(p=0,\theta\right)}{V\left(p=0,\theta_{ini}\right)}\right) \tag{18}$$

For the following considerations the liquid phase is assumed to be incompressible and its thermal expansion is ignored. The gas phase is treated as ideal gas and the process is supposed to be isotherm. Using these assumptions the volume $V(p,\theta)$ is the same as described in equation (11). Using equation (8) here leads to:

$$V\left(p,\theta\right)=\frac{\tilde{p}_{ini}*V_{G,ini}*\theta}{\theta_{ini}*\left(p_{amb}+p\right)}+V_L \tag{19}$$

Converting equation (18) the pressure and temperature dependent bulk modulus equals:

$$K\left(p,\theta\right)=-p*\left(\frac{V\left(p=0,\theta_{ini}\right)}{V\left(p,\theta\right)-V\left(p=0,\theta\right)}\right) \tag{20}$$

For a constant fluid cavity temperature θ equation (20) represents a linear relationship between the fluid cavity pressure p and the bulk modulus $K(p)$.

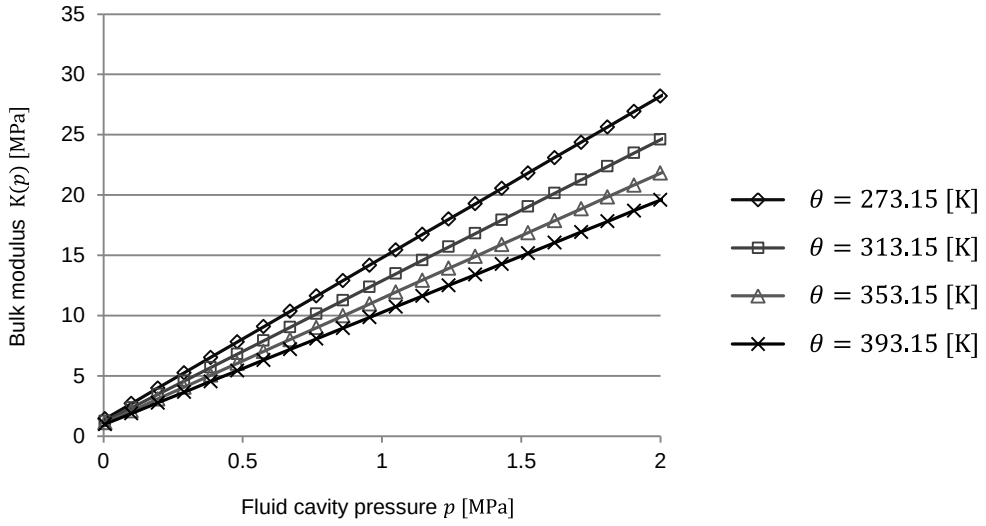

Figure 10. Bulk modulus $K(p)$ for $\tilde{p}_{ini}=p_{amb}=0.101325$ MPa, $\theta_{ini}=293.15$ K and $L_{frac,ini}=0.92$.

Figure 10 shows exemplarily the linear relation of equation (20) for a container initially filled with 92% liquid (water) and 8% gas (air).

2.2.2 Thermal expansion

Thermal expansion can be expressed in terms of the fluid density

$$\rho\left(p=0,\theta\right)=\frac{\rho\left(p=0,\theta_{ini}\right)}{1+3*\alpha\left(\theta\right)*\left(\theta-\theta_0\right)-3*\alpha\left(\theta_{ini}\right)*\left(\theta_{ini}-\theta_0\right)}, \tag{21}$$

where θ_0 is the reference temperature for the coefficient of thermal expansion and $\alpha(\theta)$ is the mean (secant) coefficient of thermal expansion (Dassault Systémes Simulia Corp., 2014).

Defining

$$\theta_0 \equiv \theta_{\text{ini}} \tag{22}$$

and reforming equation (21) leads to:

$$\alpha\left(\theta\right)=\left(\frac{\rho\left(p=0,\theta_{ini}\right)}{\rho\left(p=0,\theta\right)}-1\right)*\frac{1}{3*\left(\theta-\theta_{\text{ini}}\right)} \tag{23}$$

Equation (13) describing $\rho(p,\theta)$ can be used in equation (23) to calculate $\alpha(\theta)$. It becomes obvious that $\alpha(\theta)$ is independent of the temperature θ. It depends on the ambient pressure p_{amb}, the initial conditions θ_{ini}, p_{ini} and $L_{frac,ini}$. Figure 11 shows exemplarily $\alpha(\theta)$ for different initial conditions p_{ini} and $L_{frac,ini}$. Ambient pressure $p_{amb} = 0.101325$ MPa and initial temperature $\theta_{\text{ini}} = 293.15$ K are kept constant.

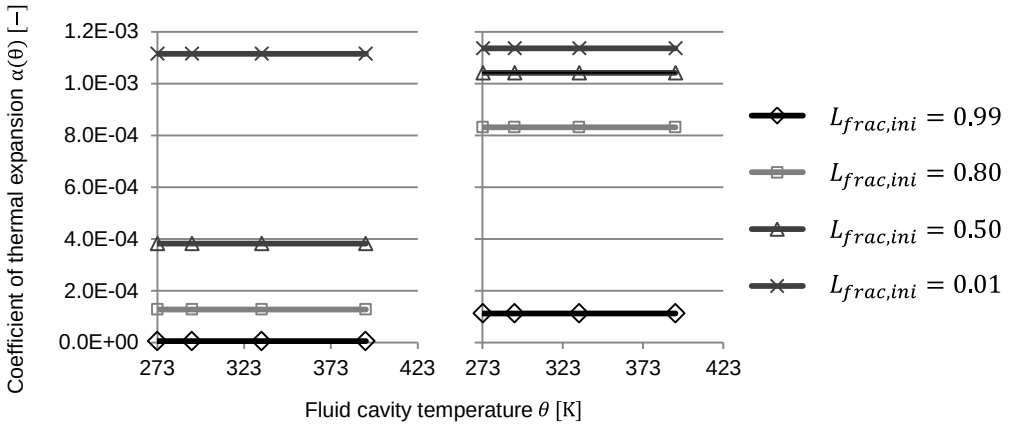

Figure 11: Coefficient of thermal expansion for different initial conditions $p_{ini} = -0.05$ MPa (left) and $p_{ini} = 1.00$ MPa (right).

2.2.3 Application of fluid properties and initial conditions to the model

The idea of the explicit approach is to take the fluid cavity pressure p_i from a converged increment i, calculate the corresponding bulk modulus $K_{i+1}(p_i)$ to be used for the following increment $i+1$.

This approach takes advantage of the possibility to include field variables into the definition of the bulk modulus in Abaqus/Standard as well as in Abaqus/Explicit. This way it is feasible to define the bulk modulus depending on a field variable representing the fluid cavity pressure. As shown in Figure 10 the bulk modulus is a linear function of the fluid cavity pressure. Hence two points of the curve are sufficient to describe the bulk modulus for a constant temperature. This definition can be completed by adding definitions for different discrete temperatures.

One can use the subroutine UAMP to define a customized amplitude representing the fluid cavity pressure as a function of time. Therefore a sensor measuring the fluid cavity pressure p is defined in the history output. The so defined amplitude is used to specify the time history of the additionally defined field variable corresponding to the field variable used in the definition of the bulk modulus as described above.

2.2.4 Verification of the method

In order to evaluate the method same model as shown in Figure 5 is used. The results from the simulation are compared with the results from simulations using the implicit approach (UFLUID) described in section 2.1. The initial conditions and the material properties are the same as in section 2.1.4.

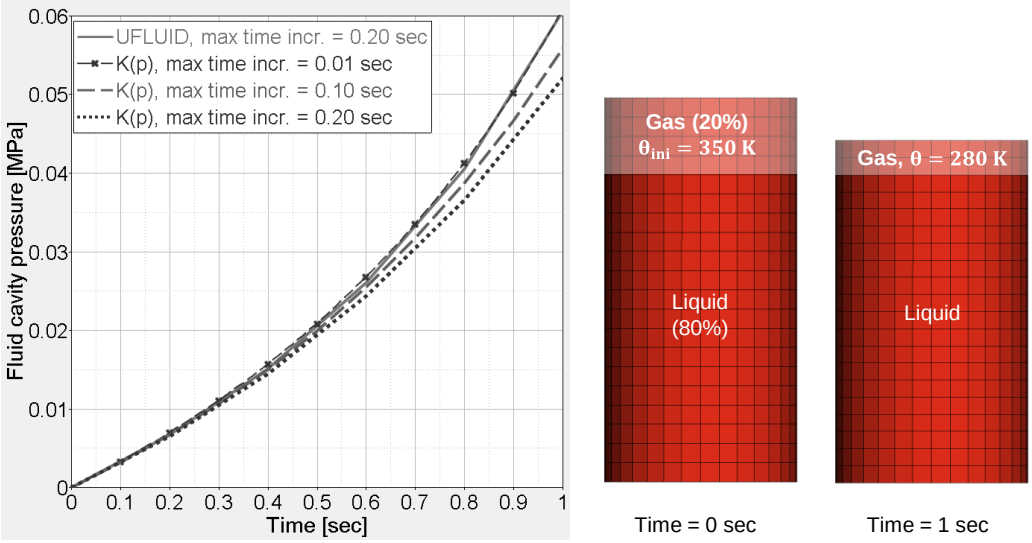

Figure 12. Fluid cavity pressure for different maximal time increments.

The explicit approach keeps the pressure dependent bulk modulus $K(p)$ constant within a time increment. Hence the choice of the maximal allowed time increment has a strong influence of the accuracy of the simulation. In contrast the implicit approach (UFLUID) considers the change of constitutive relations within the time increment.

Figure 12 shows fluid cavity pressure vs. time plots for different maximal time increments used for the explicit definition of $K(p)$. It also compares the result with the implicit approach (UFLUID). Figure 12 corresponds to case 2 as described in Table 1.

It is quite clear that for very small maximal time increments both approaches lead to the same result. As the maximal time increment increases the two approaches differ from each other.

3. Conclusions and discussion

Two approaches for modelling the two-phase system (liquid and gas) inside a partly filled and sealed container using a surface defined fluid cavity are presented – an implicit and an explicit one. The implicit approach takes advantage of user subroutine UFLUID describing the constitutive model of the two-phase system. The explicit approach uses the hydraulic fluid model of Abaqus/Standard and defines a pressure dependent bulk modulus $K(p)$ using a field variable representing the fluid cavity pressure from the last increment. To achieve this user subroutine UAMP in combination with a sensor output is needed. The background of both approaches is described and comparisons with analytical solutions for a simple model prove the accuracy of both methods.

The presented approaches consider following assumptions:

- The process is isotherm.
- The liquid phase is incompressible and its thermal expansion is neglected.
- The gas phase is considered to be an ideal gas.
- Sloshing and gravity effects of the fluid mass can be neglected.
- The initial temperature and total initial pressure (sum of ambient and initial gauge pressure) of the gas describe the reference state for density and thermal expansion.

4. References

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