Shock Wave Dynamics in the Cleaning of Container Surfaces

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Abstract— Lockable containers are commonly applied in both long-term and short-term storage of materials, substances and commodities. In repeatedly used containers, however, cleaning is a crucial problem: traces of previously stored materials have to be removed quickly and effectively, especially in the case of biological compounds or toxic, radioactive, and otherwise hazardous substances. The chemical-mechanical methods for the elimination of dirt can be excessively complicated or costly (also due to the use of special equipment), and in some materials the cleaning procedure is difficult to control

1. INTRODUCTION

In the field of material and component storage, the operators are faced with the problem of ensuring safe and repeated use of the containers. As indicated within references [1, 2], the situation is even more pressing in the context of specialised physical and chemical laboratories or plants, which apply various cleaning procedures depending on the concrete type of substance.

The authors of this paper propose a single (albeit somewhat limited) cleaning method suitable for universal application both in vessels holding nanomaterial particles and in large-sized containers with hazardous chemical or biological content. The outlined solution utilises shock wave dynamics, which — depending on the circumstances — can be obtained through a controlled electric charge or via detonation produced by a regulated chemical reaction.

2. NUMERICAL MODEL AND ITS FORMULATION

The actual creation of the numerical model is based on the laws of hydrodynamics, or the behaviour of compressible or incompressible fluids. In the given instance, the exciting detonation wave travels through the air, which (in the assumed conditions) acts as a compressible fluid; the interference of the waves at the boundary, or the container wall, nevertheless significantly changes the propagation speed of the superposed wave through the air, and this environment can be interpreted in the outlined situation as an incompressible fluid. For the definition of the model, we assume the equilibrium state, and this description forms the basis of the numerical model design. The model of the assumed task is restricted to the closed area Ω_F according to Fig. 1(a). We then have

$$\Omega_F = \bigcup_{i=1}^{4} \Omega_i \text{ a } \bigcup_{i=1}^{4} \Gamma_{\Omega i} = \Gamma_F. \tag{1}$$

From the state of the dynamic equilibrium of the system in the area Ω_F, it is possible to observe (in a simplified manner) at the boundary Γ_1 the conditions for the undamped process of an incompressible environment as the formula for the stress tensor $\overleftrightarrow{T}$

$$\mathrm{div}\overleftrightarrow{T} + \mathbf{f}_s = 0 \quad \text{in the area } \Omega_1. \tag{2}$$

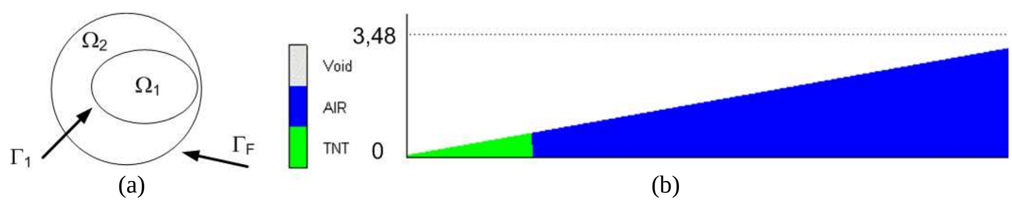

Figure 1: (a) The general distribution of areas and boundaries in the numerical model; (b) the distribution of material in the charges and the environment.

The vector of the specific force $\mathbf{f}_s$ is described by the formula

$$\mathbf{f}_s = \mathbf{f}_0 + \mathbf{f} + \rho \frac{\partial^2 \mathbf{s}}{\partial t^2}, \quad \forall t \geq 0, \tag{3}$$

where ρ is the specific density, $\mathbf{s}$ is the position vector, $t$is the time. The specific force $\mathbf{f}$ is expressed for the presence of plasma, with the magnetic flux density $\mathbf{B}$ and the current density $\mathbf{J}$, as

$$\mathbf{f} = \mathbf{J} \times \mathbf{B}. \tag{4}$$

The stress tensor from Formula (2) can be written as

$$\overleftrightarrow{T} = \overleftrightarrow{D}_F \cdot \overleftrightarrow{e} \tag{5}$$

The tensor of specific deformations is expressed as

$$\overleftrightarrow{e} = \begin{bmatrix} \frac{\partial s_x}{\partial x} & \frac{\partial s_x}{\partial y} - \frac{\partial s_y}{\partial x} & \frac{\partial s_x}{\partial z} - \frac{\partial s_z}{\partial x} \\ \frac{\partial s_x}{\partial y} - \frac{\partial s_y}{\partial x} & \frac{\partial s_y}{\partial y} & \frac{\partial s_y}{\partial z} - \frac{\partial s_z}{\partial y} \\ \frac{\partial s_x}{\partial z} - \frac{\partial s_z}{\partial x} & \frac{\partial s_y}{\partial z} - \frac{\partial s_z}{\partial y} & \frac{\partial s_z}{\partial z} \end{bmatrix}. \tag{6}$$

By substituting the stress tensor (5) and the specific force (4) in the Formula (2) and through extension, we obtain the equation

$$(\lambda_1 + \lambda_2)\, \mathrm{graddiv}\, \mathbf{s} + \lambda_2 \nabla^2 \mathbf{s} + \mathbf{f}_s = 0, \tag{7}$$

in which the Lamé constants λ_1, λ_2 are expressed for the isotropic material as

$$\lambda_1 = \frac{E_u \sigma}{(1+\sigma)(1-2\sigma)}, \quad \lambda_2 = \frac{E_u}{2(1+\sigma)}. \tag{8}$$

For the Poisson's constant σ, we have $\sigma \neq -1 \wedge \sigma \neq 0.5$, and E_u is Young's elastic modulus. This model, however, is not suitable for use in the area Ω_F, namely for the dynamics of compressible fluids with speeds over $v > 10\,\mathrm{m/s}$. The solution is unstable, and it is not of converging character in the application of either the FEM or the FVM. The physical model for the part of the area Ω_1 with an incompressible fluid from the distribution of velocities (pressures) is determined on the basis of the dynamic condition

$$\mathrm{div}\, \mathbf{v} = 0, \tag{9}$$

in the state of steady flow and considering the known distribution of the specific mass ρ

$$\mathrm{div}\, \rho\, \mathbf{v} = 0. \tag{10}$$

The fluid flow can also be described as eddy, and we then have

$$\mathrm{rot}\, \mathbf{v} = 2\omega, \tag{11}$$

where ω is the angular speed of fluid. By applying Stoke's and Helmholtz's theorems for the moving particle and the continuity equation, we formulate from the balance of forces the Navier-Stokes equation [3] for the fluid element

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \mathrm{grad}\, \mathbf{v} = \mathbf{A} - \frac{1}{\rho} \mathrm{grad}\, p + \boldsymbol{\upsilon} \cdot \Delta \mathbf{v}, \tag{12}$$

where $\mathbf{A}$ is the external acceleration, p is the pressure, $\boldsymbol{\upsilon}$ is the kinetic viscosity. In the above Equation (12), the pressure loss can be superseded by the function

$$\begin{aligned} \mathrm{grad}\, p = &-\left(K_x \rho \mathbf{v}_x |\mathbf{v}| + \frac{f_r}{D_h} \rho\, \mathbf{v}_x |\mathbf{v}| + C_x \mu_p \mathbf{v}_x\right) \mathbf{u}_x - \left(K_y \rho\, \mathbf{v}_y |\mathbf{v}| + \frac{f_r}{D_h} \rho \mathbf{v}_y |\mathbf{v}| + C_y \mu_p \mathbf{v}_y\right) \mathbf{u}_y \\ &-\left(K_z \rho\, \mathbf{v}_z |\mathbf{v}| + \frac{f_r}{D_h} \rho\, \mathbf{v}_z |\mathbf{v}| + C_z \mu_p \mathbf{v}_z\right) \mathbf{u}_z \end{aligned} \tag{13}$$

where K represents the locally restricted pressure forces, f_r is the drag coefficient, D_h is the hydraulic radius, C is the transmissivity of the system, μ_p is the fluid dynamic viscosity, $\mathbf{u}_x$, $\mathbf{u}_y$, $\mathbf{u}_z$ are the unit vectors of the Carthesian coordinate system. The drag coefficient can be substituted with a function from the Blasi formula

$$f_r = aR_e^{-b}, \tag{14}$$

in which the coefficients a, b are determined according to reference [4], and R_e is the Reynolds number. The above-described model can be further solved using again the finite element or the finite volume methods (FEM; FVO). Their main limitation can be identified in the necessity to correctly formulate the dependence of instantaneous values of velocity $\mathbf{v}$ $(x,\ y,\ z,\ t)$ on time and space, and their major advantage consists in the evaluation accuracy and solution stability in the time domain. In the search for the convergent system, we tested various approaches based on ANSYS, SFX and DYNA [6]. For the FVM, it is possible to expect here a converging solution up to the mean velocity having the maximum of 150 m/s, as previously obtained from the CFX program. The ANSYS tool uses, at speeds of $Ma > 3$ for the compressible environment at the boundary between the wall and the fluid, the Van Driest transformation

$$U_{com,x,y,z} = \frac{u_\tau}{\kappa} \ln\left(\frac{y^* y}{\upsilon}\right) + C \tag{15}$$

where $U_{com,x,y,z}$ is the logarithmically expressed speed of the compressible medium wave, u_τ is the velocity in the transverse direction, κ is the constant, y is the distance from the wall, υ is the specific volume, C is the constant. Another option consists in applying the shock load method [5], which is known from its use with solid states and compressible fluids. Major attention has to be paid to the model of the material, considering the following aspects:

1. elastic deformation (v_d — the speed of incidence; D — the load intensity), $v_d \approx 1$ m/s, $D \approx 10^{-5}$.
2. beginning of plastic deformation, $v_d \approx 10$ m/s, $D \approx 10^{-3}$.
3. plastic deformation, $v_d \approx 100$ m/s, $D \approx 10^{-1}$.
4. intensive plastic deformation, $v_d \approx 1000$ m/s, $D \approx 10^{+1}$.
5. phase and chemical variations in the material, $v_d \approx 10000$ m/s, $D \approx 10^{+3}$.

To facilitate successful creation and solution of the model, a higher number of stability conditions have to be applied during the formulation of the physical model. Thus, it is convenient to use the law of conservation of mass, the law of conservation of momentum, and the law of conservation of energy. These physical models are then converted to a mathematical model in the form

$$[M_F]\left\{\ddot{S}\right\} + [C_F]\left\{\dot{S}\right\} + [K_{F1} - K_{F2}]\{S\} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -K_{F5} & K_{F4} & -K_{F3} & K_{Fe} \end{bmatrix} \begin{Bmatrix} F \\ p_\sigma \\ p_n \\ E_{Te} \end{Bmatrix}, \tag{16}$$

where M_F, C_F, K_{F1}, K_{F2}, K_{F3}, K_{F4}, K_{F5}, K_{Fe} are the coefficients of the systems of equations of the LS Dyna module (the ANSYS tool) [6], S is the discrete nodal values of the displacement vectors. The entire solution is carried out via the explicit method for transient analysis, whose closer description can be found in reference [6]. The model of the physical approach is best described within source [7] as a dynamic model of viscous fluids. This model is based on dynamic stability of the system and complemented with the laws of conservation of mass, momentum, and energy; the formulation is known as the dynamic equilibrium equation, and its structure can be obtained via combining the Equations (2) and (3).

$$\rho\frac{dv}{dt} = f_s + div\overleftrightarrow{T} \quad \text{in the area } \Omega_F. \tag{17}$$

3. ANALYSIS AND EVALUATION OF THE NUMERICAL MODELS

The geometry and distribution of the materials are shown in Fig. 1(b). The unlimited model representing the propagation of the detonation and the pressure wave was analysed as a 1D task. For the model of the explosive, we used the TNT agent in an elongated charge having the diameter of 8 mm. The air was included up to the distance of 200 mm. Subsequently, the resulting pressure wave was transferred to a 2D model, which was carried out using the AUTODYN 2D tool; the results of the analysis are presented in Fig. 2 for the time interval of 0–200 µs from the beginning of the detonation. Here, the interpreted analysis of the pressure field distribution is presented. At the moment the wave front reflects from the walls of the container, the interference of the waves and the wave propagation on the surface of the container wall will occur.

When designing a system for the cleaning of small-size containers whose dimensions range between 0 µs and 10 cm, we can act on the container walls by utilising the properties of an electric discharge and creating a detonation wave through a controlled process. This method is characterised by several advantageous aspects, above all repeatability and safe formation or shaping of the detonation wave via electronic circuits. Thus, the described technique is suitable for use in demanding applications, for example the removal of nanoelements, which may stick to the container wall and are difficult to identify. In the given context, the proposed approach can also be suitably utilised to eliminate materials chemically unsafe of consisting of multiple biological structures. In containers with dimensions ranging between 100 cm and 10 m, it is possible to exploit the chemical reactive and formation processes related to detonation. An example of such technology consists in solidifying towers. To describe solidification as a waste material conversion process, let us refer to the object in Fig. 3, in which the flue ash obtained after the first stage of combustion product cleaning is mixed with the output of the second stage of purification; water and cement are used as the binding agents.

At present, solidifying towers are cleaned either mechanically (Fig. 3(b) or chemically. In Fig. 3(c), we present the use of blasting technics for the decontamination of solidifying towers. The intensity of the shock wave I is directly proportional to the initial energy ΔE and indirectly proportional to the propagation plane S, considering a spherical plane. $I = \Delta E/S$, where $S = 4\pi \cdot l_2$,

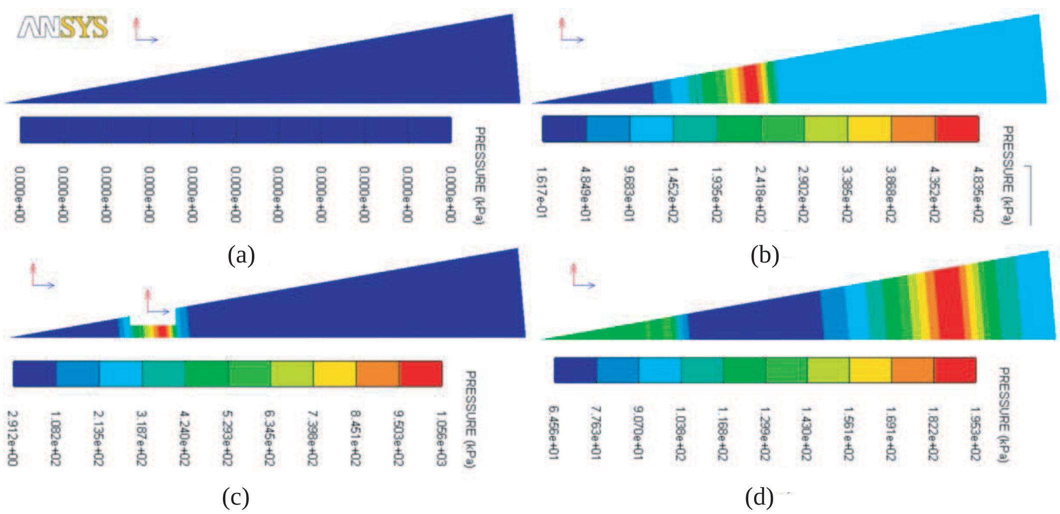

Figure 2: (a) The initial pressure state $p(t)$, $t = 0$. (b) The pressure distribution $p(t)$, $t = 30$ µs. (c) $p(t)$, $t = 60$ µs. (d) $p(t)$, $t = 195$ µs.

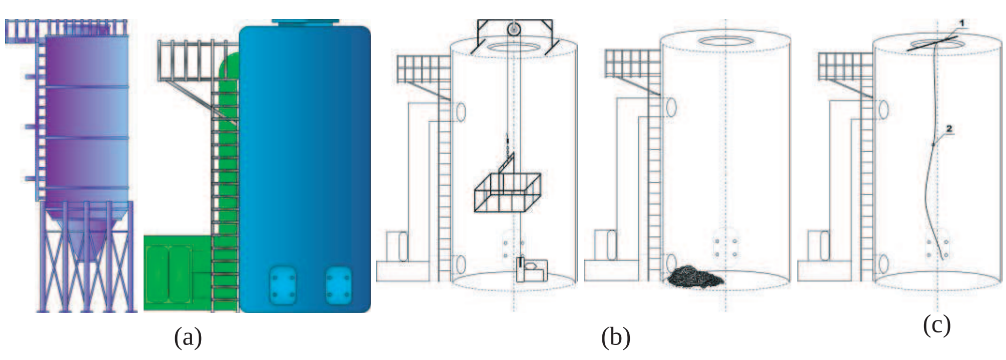

Figure 3: (a) A solidifying tower. (b) Mechanical cleaning of a solidifying tower. (c) Cleaning process using an elongated charge.

in which l_2 is the distance of the direct detonation line 1 from the location of the detonation origin. The actual cleaning process exploits the energy of a shock wave. The shock wave induced by the blast of an explosive charge acts both on obstacles in its path and on the environment through increased pressure and via the related dynamic forces. This reaction can be utilised in reducing the unfavourable effects upon the container wall during the interference of shock waves generated by smaller charges.

The interference of two circular or spherical waves, Fig. 4, occurs as a product of the burning of two charges located at an ample distance from each other. An interfered wave develops within this process, and the resulting split waves propagate from both sources simultaneously against one another. Here, the aim is to acquire identical waveforms of the waves in time; in this state, the waves oscillate with the same phase. The obtained superposed wave will create a reflected component, Fig. 4, which propagates in the opposite direction at a speed up to 26-fold higher. Such a speed value constitutes the double of the value of the reflexive pressures.

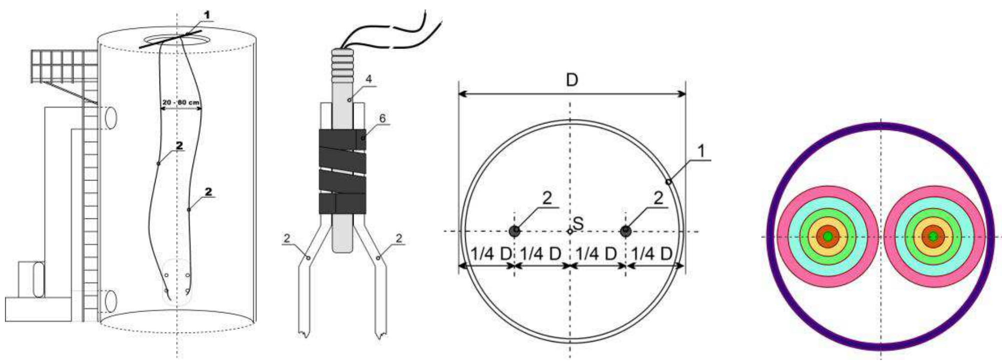

Figure 4: The arrangement of two elongated charges and the shock wave propagation.

4. CONCLUSION

The described technique of shock wave generation ensures a higher efficiency rate in the cleaning of container surfaces. In small-sized containers, the desired detonation waves can be obtained via various physical processes or phenomena, for example through controlled electric charges in the air or another applicable gas.

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