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A particle-based approach to close-range blast loading

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Abstract

A new approach to describe blast loading is suggested, herein referred to as the corpuscular approach. The detonation products are modeled as a set of discrete particles following Maxwell's original kinetic molecular theory. For numerical purposes, the number of molecules has to be greatly reduced compared to what one has in real gases. However, the total molecular mass and temperature dependent velocity distribution are the same as in an ideal gas. Pressure loading on structures is then numerically represented by the momentum transfer as particles impact and rebound from the surface of the structure. The suggested approach has significant advantages compared to today's state of the art continuum-based approaches to fully coupled blast-loading computations. The computational time can be significantly reduced, the method is numerically robust and the approach will easily cope with complex geometries in the fluid-structure interface.

Key words: Blast loading, fluid-structure interaction, kinetic molecular theory

1. Introduction

Until recently, continuum-based Eulerian approaches have been regarded as the most accurate technology for finite element airbag deployment simula-

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tions. However, a continuum based approach to the modeling of airbag gases and their interaction with the airbag fabric is subjected to several difficulties. One major problem is that there are geometrical complexities that are hard to handle, both in the gas-fabric contact and in the treatment of gas flowing through narrow gaps.

As an attempt to circumvent those difficulties, a corpuscular method for gas dynamics has been developed (Olovsson 2007). The corpuscular approach is based on Maxwell's kinematic molecular theory (Maxwell 1860) and it is implemented in the non-linear, explicit finite element code LS-DYNA (LSTC 2007). The method is Lagrangian, which simplifies the gas-fabric contact treatment. It was further observed that the particle method is extremely robust and less CPU demanding than the Eulerian approaches.

Also for close-range blast loading applications, such as the description of a mine explosion underneath a vehicle, complex geometries may need to be considered. This type of simulations are known to be very CPU-demanding when using a fully coupled Eulerian approach, see e.g. (Børvik et al. 2008). It is therefore the objective of the current work to investigate whether the recently implemented corpuscular method can be utilized in its present form to also describe close-range blast loading. It is clear that certain limitations apply to the method in its current form when used to describe the detonation products. Firstly, the approach is based on an ideal gas assumption that deviates from the equations-of-state that usually are used to describe blast loading, e.g. JWL EOS (Dobratz and Crawford 1985). Secondly, the method is dispersive which means that elastic waves are quickly smeared out. **The dispersion is caused by a particle mean-free-path that is several orders of magnitude larger than the molecular mean-free-path in a real gas**.

The approach is thus likely best suited to describe close-range blast loading events. Note that several numerical studies on blast loading of structures, using various numerical approaches, have been presented in the literature over the years. A limited state-of-the-art of some recent publications can be found in **(Børvik et al. 2008)**.

In this study, Section 2 gives an overview of the corpuscular approach, based on (Olovsson 2007). An experimental set-up used by (Neuberger et al. 2009) is briefly described in Section 3. This set-up is used as basis for a comparison between the Eulerian and corpuscular approaches in Section 4. In the Eulerian case the high explosive has been modeled both as an ideal gas and with the JWL equation-of-state.

2. Overview of the corpuscular approach

The corpuscular method is essentially based on the kinetic molecular theory, with some deviations to allow for a numerical treatment of gas volumes on a macroscopical level.

2.1. Kinetic molecular theory

The kinetic molecular theory is the study of gas molecules and their interaction (on a microscopic level) which leads to the ideal gas law (macroscopic relationships). The theory is based on the following assumptions:

- The average distance between the molecules is large compared to their size.
- There is a thermo-dynamical equilibrium, i.e. the molecules are in random motion.
- The molecules obey Newton's laws of motion.
- The molecule-molecule and molecule-structure interactions are perfectly elastic collisions.

The kinetic molecular theory dates back to 1738 when Daniel Bernoulli (Bernoulli 1738, 1968) proposed a theory that the air pressure against a piston is built up by discrete molecular collisions. Having the kinetic theory as a starting point James Clerk Maxwell (Maxwell 1860) derived a very elegant expression for the molecular velocity distribution at thermal equilibrium

$$f(v) = 4\pi \left(\frac{M}{2\pi RT}\right)^{3/2} v^2 \exp\left[\frac{-Mv^2}{2RT}\right]. \tag{1}$$

Here $f(v)$ is the probability density function for the molecular velocity. M is the molar mass, R is the universal gas constant and T is the temperature. As an example Figure 1 shows the velocity distribution of CO_2 at thermal equilibrium at 500K and at 1000K. The root-mean-square velocity at thermal equilibrium can be calculated as

$$v_{rms} = \sqrt{\int_0^\infty v^2 f(v) \mathrm{d}v} = \sqrt{\frac{3RT}{M}}. \tag{2}$$

v_{rms} is a thermal velocity and it should not be mixed up with the flow velocity. As an example, the molecules in air at room temperature have a root-mean-square velocity of roughly 500m/s. The normal atmospheric pressure is built up by molecules that collide with the surroundings, most of them with a velocity of several hundreds of meters per second.

Maxwell managed to bring more understanding to details about the molecular interaction in an ideal gas. One can, from his statistical descriptions, derive quantities such as the mean-free-path, l

$$l = \frac{1}{\sqrt{2}\pi n r_p^2} \tag{3}$$

and frequency of collision, f_c

$$f_c = n r_p^2 \sqrt{\frac{8\pi RT}{M}} \tag{4}$$

where r_p is the molecular radius and n is the number of molecules per unit volume.

2.2. Corpuscular method as implemented in LS-DYNA

Depending on the molecular weight one can expect somewhere in the order of $10^{22} - 10^{23}$ molecules for each gram of detonation products. Hence, one can not possibly model every single molecule in a full scale blast scenario. The need for computational efficiency in the numerical implementation has lead to the following assumptions and deviations from the kinetic gas theory:

- **The particles are rigid and they are given a spherical shape (speeds up contact treatment).**
- Each particle represents many molecules, typically $10^{15} - 10^{20}$ depending on application.
- For each individual particle there is a balance between translational kinetic energy, W_t, and spin/vibration energy, W_s. This balance is determined directly from $\gamma = C_p/C_v$, where C_p and C_v are the heat capacities at constant pressure and volume, respectively. The balance is assumed as **(Olovsson 2007)**

$$\frac{W_s}{W_t} = \frac{5 - 3\gamma}{3\gamma - 3} \tag{5}$$

It is to be noted that, in a cloud of real molecules, the ratio between spin/vibration and translational energy is a statistical property. It is not valid for every single molecule individually.

The defined ratio between W_s and W_t is based on the assumption of thermal equilibrium. This is a realistic assumption for most airbag applications, but not in blast simulations where the gas flow velocity is extremely high.

- W_s is a lumped scalar variable for each particle. Hence, the particles are not assigned any degrees of freedom for the spinning/vibration.
- As a particle impacts a moving structure W_t will change, while W_s is assumed unaffected. Hence, the correct ratio between W_s and W_t will be disrupted.
- As two particles collide their energies are redistributed to restore, or maintain, a correct ratio between W_s and W_t. This is done in a way that ensures both the total energy balance and the momentum balance.
- **The particle radius is adjusted dynamically to obtain a reasonable mean-free-path. The mass is kept constant though. A too small radius will lead to an inability of transferring pressure waves. A too large radius, on the other hand, makes the gas behavior deviate from the ideal gas law. In addition the particle-particle contact calculation will become computationally more expensive as the particle size grows.**

3. Reference test set-up

The evaluation example is taken from (Neuberger et al. 2009), where a clamped circular RHA steel plate is exposed to the blast loading from a 15kg TNT charge with stand-off distance 1m, see Figure 2. The details from the experimental study and the experimental results can be found in (Neuenberger et a. 2009) and will therefore not be repeated here. However the peak deflection of the plate during the blast was estimated to be 34mm. This value will be used in the validation of the numerical results in the next section.

The rate dependent hardening model for the steel plate has been taken directly from (Neuberger et al. 2009).

$$\sigma_y = \left(\sigma_0 + E_p \epsilon_{eff}^p\right) \left[1 + \left(\frac{\dot{\epsilon}}{D^*}\right)^{1/q}\right] \tag{6}$$

where σ_0 is the initial yield stress, E_p is a constant hardening modulus, ϵ_{eff}^p is the effective plastic strain and $\dot{\epsilon}$ is the total strain rate. D^* and q define the strain rate effects, i.e. the Cowper-Symonds model (Jones 1989). The material parameters used in the simulations are given in Table **??**.

4. Eulerian versus corpuscular method

An Eulerian and a corpuscular model of the test set-up were prepared where 1/4 of the plate and 1/8 of the charge was modeled, see Figure 3. The Eulerian model was run with four different element sizes (Δx = 1/2, 1, 2 and 4cm) and the corpuscular model with three different number of particles ($N_p = 10^4, 10^5$ and 10^6).

In the Eulerian case a spatially second order accurate advection scheme was used (van Leer with half index shift (HIS) for the momentum).

4.1. High explosive using the JWL equation-of-state

It was decided to first run the Eulerian models using the JWL equation-of-state for the high explosive. The purpose it to obtain results that may serve as a reference when evaluating the ideal gas simulations. The JWL equation-of-state expresses the pressure as a function of relative volume and internal energy according to

$$p = A\left(1 - \frac{\omega}{R_1 V}\right) \mathrm{e}^{-R_1 V} + B\left(1 - \frac{\omega}{R_2 V}\right) \mathrm{e}^{-R_2 V} + \omega e \tag{7}$$

where A, B, R_1, R_2 and ω are the JWL parameters, see Table **??**. Note that the relative volume $V = \rho/\rho_0$ is the fraction of the current and initial densities and e is the internal energy per unit volume. Table **??** also gives the detonation velocity D and the initial internal energy per unit volume e_0.

4.2. Air and high explosive as ideal gas

The ideal gas law can not capture the sharp pressure drop during adiabatic expansion that a real high explosive will undergo. The main reason is the neglecting of co-volume effects **(Baibuz et al. 1985), (Clausius 1880)**. In an attempt to match the high explosive pressure-volume relationship as accurately as possible, one should pick an as large γ as possible. In this work γ was set to 5/3. This corresponds to a mono-atomic gas and it is the theoretically largest value that one can have.

One important feature of mono-atomic gases is that no energy is stored as vibration or spin. Hence, the erroneous assumption of thermal equilibrium when defining the ratio between W_s and W_t has no negative effect on the accuracy as long as $\gamma = 5/3$.

The material parameters for the detonation products and the air are given in Table **??**, where ρ_0 and e_0 are the initial gas density and internal energy per unit volume, respectively.

4.3. Defining the particle radius

In this work r_p was dynamically adjusted (spatially and in time) such that the particles occupy 20% of the space. That is

$$n(\mathbf{x})\frac{4\pi r_p^3(\mathbf{x})}{3} = 0.2 \tag{8}$$

where $\mathbf{x}$ is a spatial coordinate and $n(\mathbf{x})$ is the local number of particles per unit volume. The 20% fill fraction has, through an empirical study in this work, proven to produce the most accurate results. A smaller radius will increase the dispersion of the pressure wave and a larger radius increases the co-volume effects to an unacceptable level. **These findings are preliminary and a more detailed study needs to be conducted in the future.**

4.4. **Initial particle velocity distribution**

The particles are injected into the model through a set of point sources. It takes about 2ms for the particles to reach thermal equilibrium. At thermal equilibrium, the velocity distribution follows Equation (1), with the relationship between translational energy and spin/vibration according to Equation (5).

The high pressure detonation products are separated from the air by a rigid shell membrane. Upon reaching thermal equilibrium, the pressure wave is released by suddenly removing this structure.

4.5. Boundary conditions

There is a 1atm external pressure applied to the boundaries of the particle domain. Particles reaching the boundary are allowed to leave the domain if the local pressure is above 1atm. At pressures below 1atm, particles are forced to bounce back.

4.6. Results

The blast process was followed for 3ms after detonation and all simulations were carried out using one AMD Opteron processor.

The corpuscular simulation results are not easily visualized. The method is not based on continuum mechanics and, hence, there are no solution variable fields that one can plot. As currently implemented in LS-DYNA one will only see a cloud of points defining the current particle locations, see Figure 4.

Table **??** lists some of the simulation results. It is to be noted that the tested numerical methods predict a smaller peak deflection than observed in the experiments. The presented CPU times for the corpuscular simulations only include the time after releasing the pressurized gas. The initialization process is omitted. The gas needs to be injected to the computational domain through a set of point sources. This is a very inefficient way to initialize large volumes with gas at thermal equilibrium. A random distribution of particles would take no more that a few seconds to achieve, but this feature remains to be implemented in LS-DYNA.

The accumulated impulses versus time that are being transferred to the target plate are shown in figures 5 and 6. The corpuscular method seems less sensitive to the model size (number of degrees of freedom) than the Eulerian approach. A coarse model even produces a larger impulse than a fine one. The corpuscular method is Lagrangian and, hence, does not suffer from the advection related dissipation errors that one experiences with an Eulerian formulation. It is also noticeable that the JWL equation-of-state produces a significantly lower impulse and a slightly smaller deflection than the ideal gas model. Figures 7 and 8 show the plate center deflection as function of time.

5. Conclusions

This initial study shows that the corpuscular method has the potential to become a very useful tool for simulating close range blast effects on structures. The method is numerically robust, relatively fast and easy to use. Further, the results from the corpuscular method seem to be in good agreement with corresponding Eulerian simulation results and available experimental data.

However, the current implementation in LS-DYNA lacks several features and further development is needed before the method can be used in production:

- The method must be improved to account for co-volume effects. This is necessary in order to better match the expected pressure-volume relationship at high densities.
- The current initialization procedure require all gases being injected through point sources. In this study it actually took more CPU time to initialize the model and to reach thermal equilibrium than it took to simulate the blast event.
- The assumption of thermal equilibrium when defining the ratio W_s/W_t is not acceptable. Currently, only mono-atomic gases can be modeled accurately enough.
- The detonation process and transformation from solid state to a gas is currently not taken into account.
- The definition of the particle radius needs to be analyzed and adapted for blast simulations.

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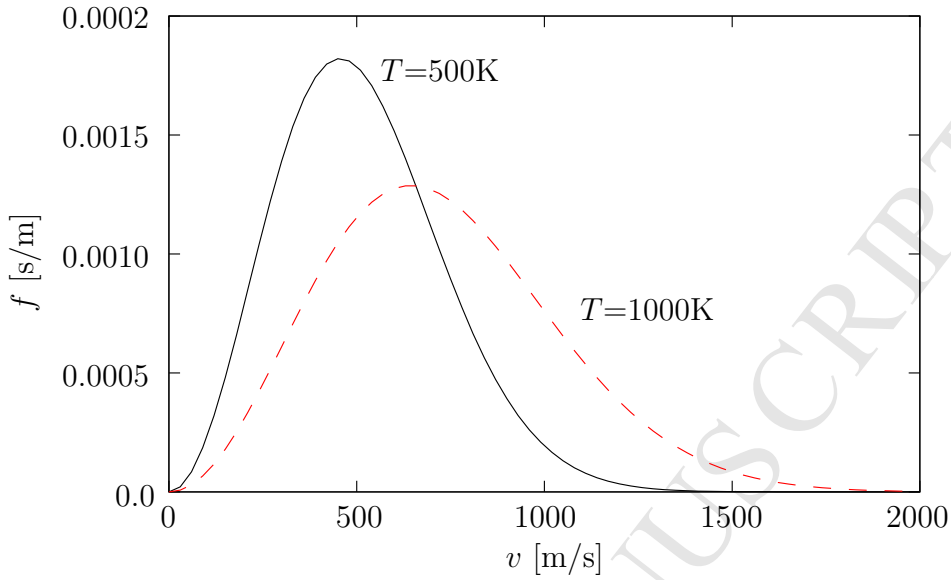

Figure 1: Velocity distribution of CO_2 at thermal equilibrium.

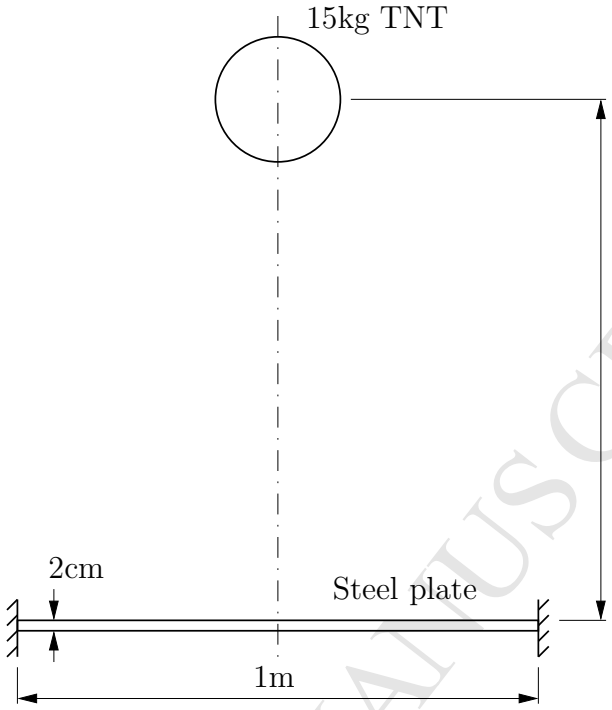

Figure 2: Axi-symmetric reference test set-up

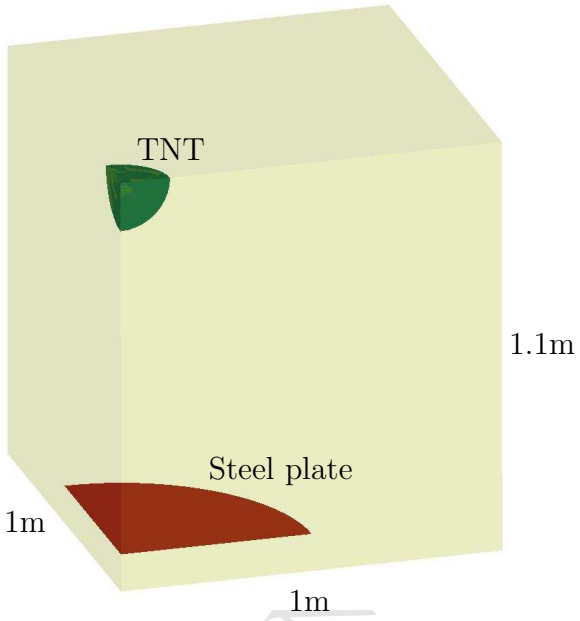

Figure 3: Modeled domain in Eulerian and corpuscular simulations.

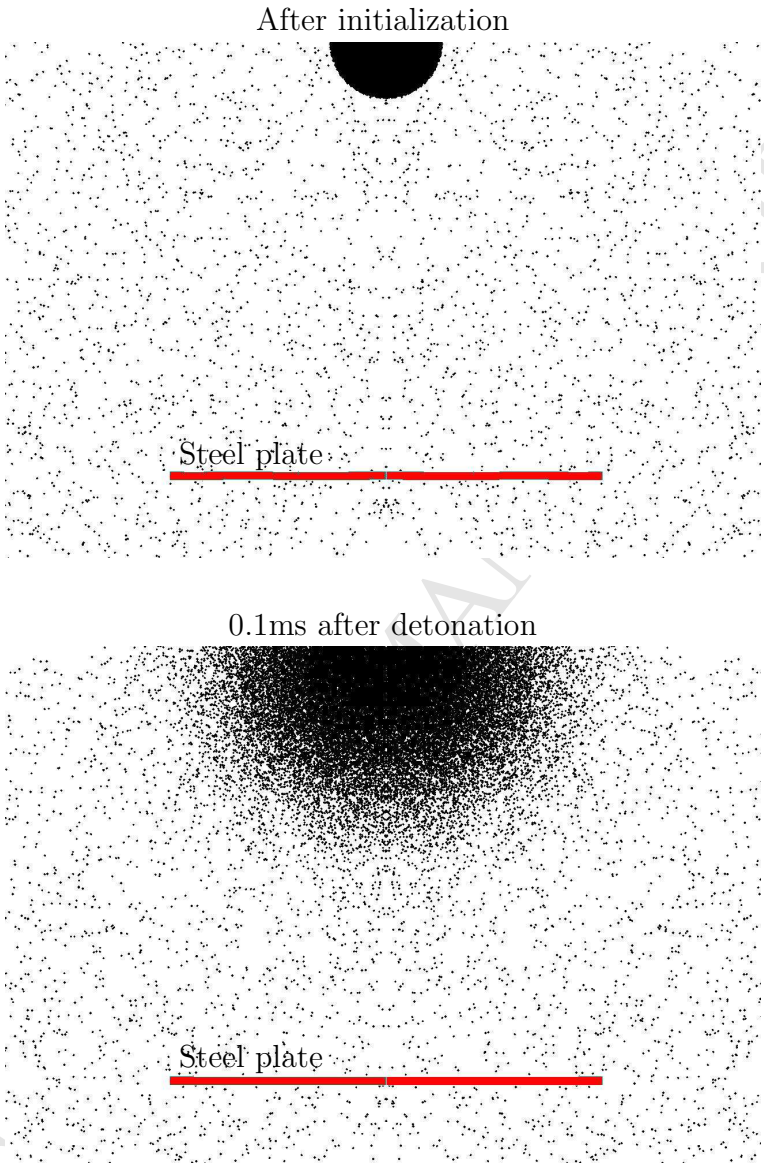

Figure 4: Corpuscular simulation with 10^4 particles after initialization and 0.1ms after detonation.

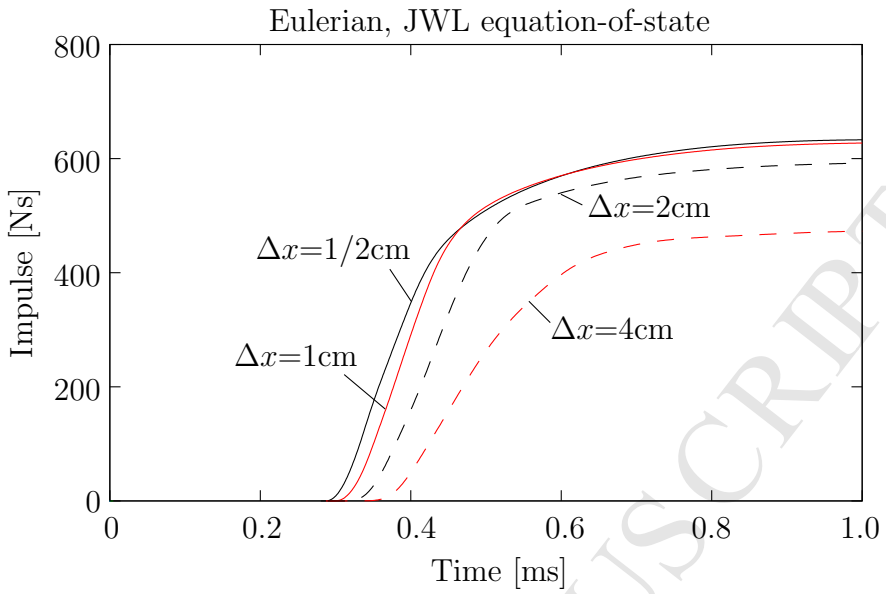

Figure 5: Impulse transferred to plate, modeling the high explosive with the JWL equation-of-state.

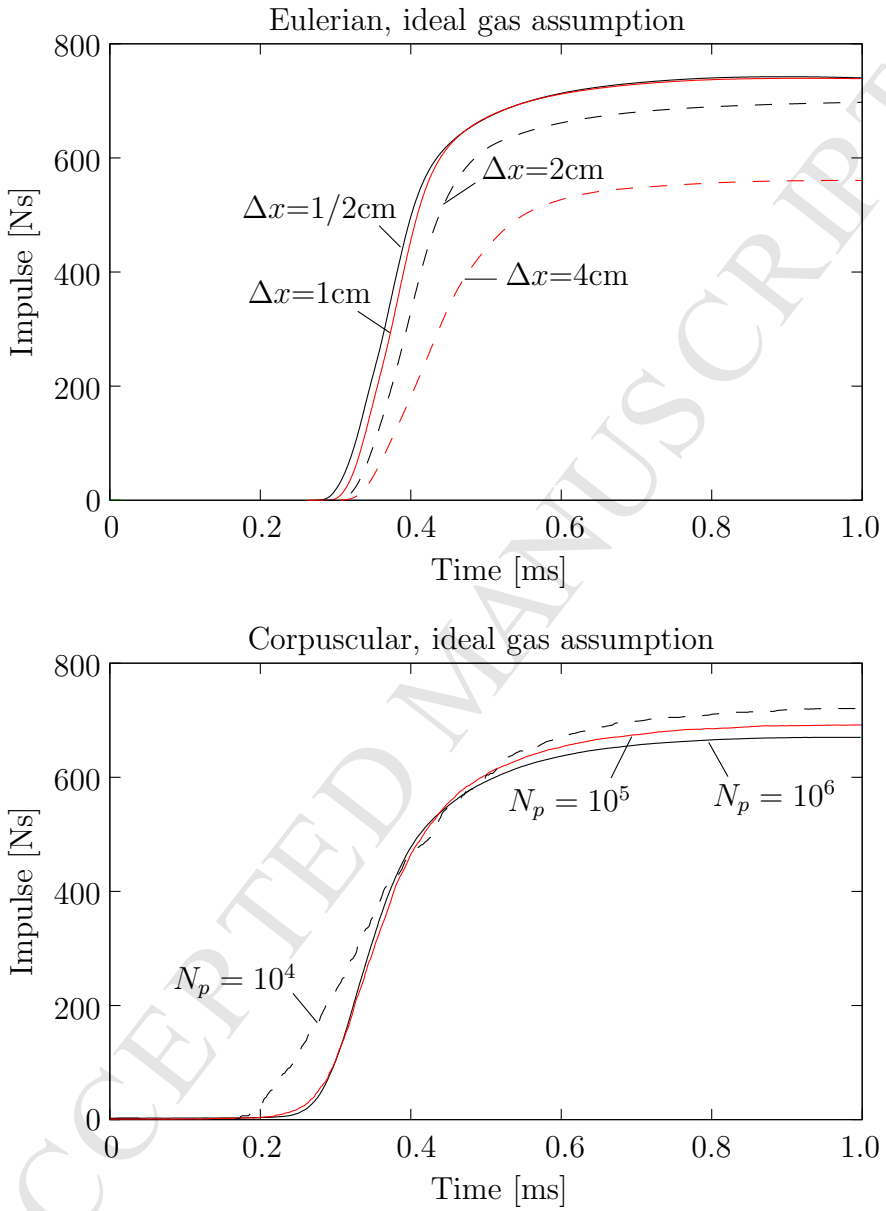

Figure 6: Impulse transferred to plate, modeling the detonation products as an ideal gas

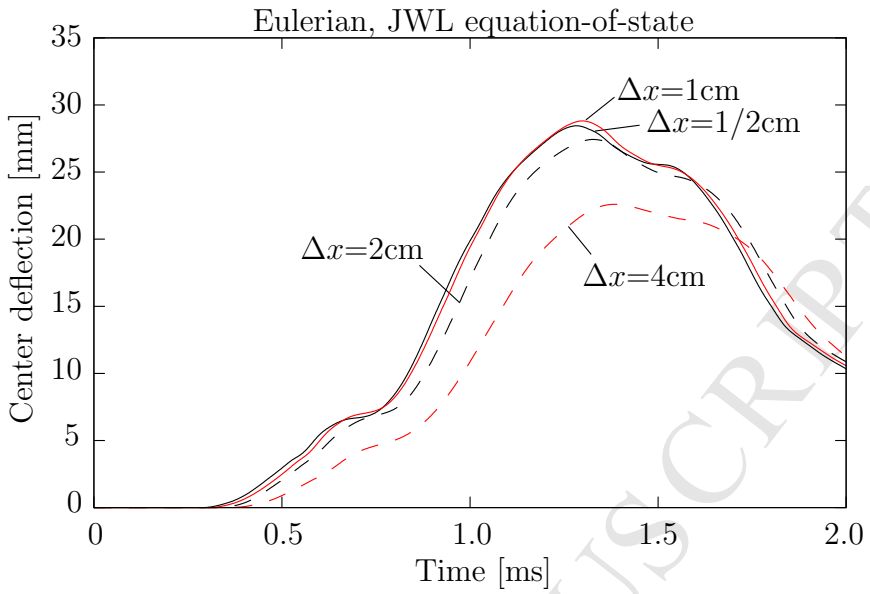

Figure 7: Center deflection versus time, modeling the high explosive with the JWL equation-of-state.

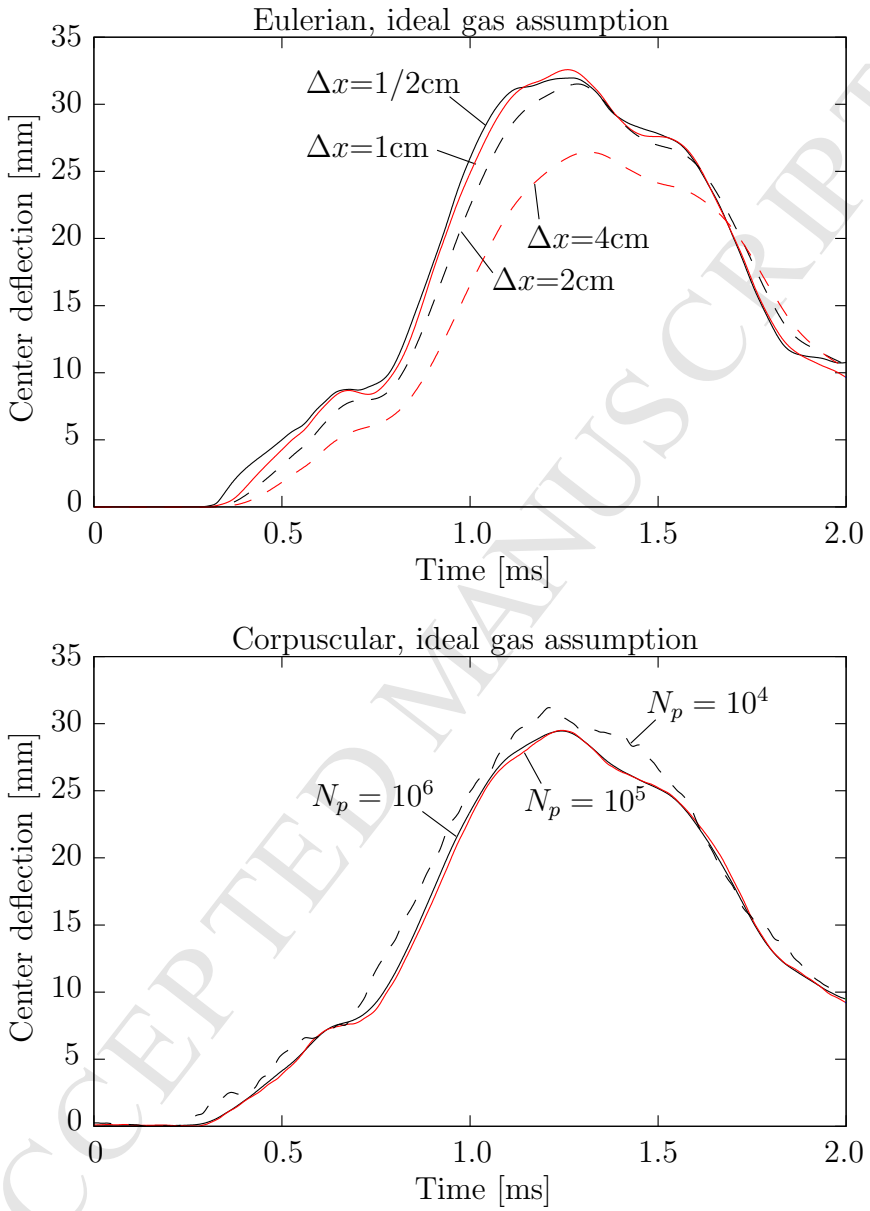

Figure 8: Center deflection versus time, modeling the detonation products as an ideal gas

Table 1: Material properties of the RHA steel plate.

σ_0 [MPa]	E_p [MPa]	D^* [s^{-1}]	q [–]
1200	6500	300	5

Table 2: Properties of TNT charge when using JWL equation-of-state.

D [m/s]	p_{CJ} [GPa]	A [GPa]	B [GPa]	R_1 [-]	R_2 [-]	ω [-]	ρ_0 [kg/m^3]	e_0 [J/m^3]
6930	21	371.2	3.231	4.15	0.95	0.3	1630	$7 \cdot 10^9$

Table 3: Properties and initial state of air and detonation products.

	γ [−]	ρ_0 [kg/m^3]	e_0 [J/m^3]
Air	1.4	1.27	$2.53 \cdot 10^5$
HE	5/3	1630	$7 \cdot 10^9$

Table 4: Simulation results. The peak deflection in the experiments (Neuberger et al. 2009) has been estimated to 34mm (measured in diagram).

Eulerian, JWL

Δx [cm]	Impulse [Ns]	Peak deflection [mm]	CPU time [s]
4	474	22.6	103
2	593	27.4	2231
1	628	28.8	52521
1/2	633	28.4	501651

Eulerian, ideal gas

Δx [cm]	Impulse [Ns]	Peak deflection [mm]	CPU time [s]
4	560	26.5	114
2	702	31.5	981
1	739	32.6	47970
1/2	742	32.0	744760

Corpuscular, ideal gas

N_p [−]	Impulse [Ns]	Peak deflection [mm]	CPU time [s]
10^4	711	31.2	55
10^5	693	29.5	562
10^6	671	29.5	2228