An open source tool for calculating CO_2 pipeline decompression wave speed

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Abstract. This paper describes the calculations required to estimate the pipeline decompression velocity based on a rigorous equation of state for pure CO_2 and mixtures with significant impurities.

Introduction

Various tools has been presented in the literature for simple calculations of the decompression wave speed such as GASDECOM [1], EPDECOM [2] and DECOM [3], which employ the assumption unidimensional isentropic, homogeneous equilibrium and inviscid formulation of the decompression wave without explicitly solving the fluid transport equations [4]. On the other end of the scale various 1-D/2-D CFD based tools have also been demonstrated where the mass, momentum, and energy balances are explicitly solved [5, 6, 7]. Common to all tools is that some are purely academic and some have been developed into commercial products. However, none of the aforementioned tools are freely available to the public. In that respect, the tool presented in the present paper differentiates itself from these tools: it is open source and freely available for use by the public.

1 Methods

1.1 Decompression wave speed

In RAMDECOM the calculation methodology for the decompression wave speed follows that shown in [8, 9]. When assuming the decompression wave to be isentropic, in homogeneous equilibrium and inviscid, the decompression wave speed, W, is expressed as:

$$W = C - U \tag{1}$$

where C is the fluid speed of sound and U is the fluid outflow velocity. The outflow velocity is given at any pressure, P, by:

$$U = -\int_{P_0}^{P} \frac{C d\rho}{\rho} = -\int_{P_i}^{P} \frac{dP}{C\rho} \tag{2}$$

where P_0 is the initial pressure and ρ is the fluid density. Integration is performed along an isentropic path. The outflow velocity in the above equation can be expressed by numerical integration using finite difference:

$$U_i = U_{i-1} + \frac{P_{i-1} - P_i}{C_i \rho_i} \tag{3}$$

where the subscript i refers to the current integration step and $i-1$. Properties from the previous step is known, only density and speed of sound needs evaluation at the new step.

In order calculate the density and the speed of sound, as well as VLE behaviour, an adequate equation of state is required. In the currect work CoolProp [10] or REFPROP [11] is used as the thermodynamic backend. Both tools use Helmholtz energy formulations for fluids modelling both for pure fluids and for mixtures. For pure CO_2 the Span-Wagner equation of state is employed [12], for mixtures the method of Lemmon [13] and Kunz [14] is used. For mixtures with CO_2 the binary parameters in both CoolProp and REFPROP have been updated with those from EOS-CG [15] and later estimations by Herrig [16].

While the speed of sound is well defined for a single phase fluid, further assumptions are required in order to define it for two-phase / multi-phase. Assuming homogeneous equilibrium the speed of sound can generally be defined as:

$$C = \sqrt{\left(\frac{dP}{d\rho}\right)_s} \approx \sqrt{\left(\frac{P_{i-1} - P_i}{\rho_{i-1} - \rho_i}\right)} \tag{4}$$

where the differential is evaluated at isentropic conditions. The full calculational workflow is the following:

- Define initial conditions: T_0, P_0 and composition (either pure CO_2 or mixture with impurities)
- Calculate density and specific entropy using the equation of state
- For each integration step from the initial pressure the new pressure P_i is set as P_{i-1} + 1e5 Pa and new density is evaluated via an isentropic path.
  - The speed of sound, C_i, is calculated via Eqn. 4 assuming a small ΔP of 100 Pa.
  - C_i is used in Eqn.3 to calculate the outflow velocity U_i
  - W_i is calculated using Eqn. 1

The calculations are generally continued until the calculated decompression wave speed becomes zero or negative. The evaluation of properties and estimation of speed of sound is performed at specified pressure and entropy (equal to the initial entropy) i.e. a PS-problem.

For all calculations the CoolProp python wrapper is used. When using REFPROP as backend this is done still via the CoolProp wrapper. The CoolProp backend is applied only for pure CO_2, since the two-phase mixtures failed to solve in many cases. REFPROP can be specified both for pure CO_2 and for mixtures. This work is a continuation of a previous work [17] with the purpose of building useful engineering tools on top of high quality open source software packages. RAMDECOM is developed entirely in python 3 and also relies on other python packages such as pandas [18], matplotlib [19], and numpy [20].

1.2 Experimental

In order to compare the presented decompression model with experimental data various relevant experiments have been sourced from the literature. For decompression of pure CO_2 experiments made by Munkejord *et al.* [21] and Botros *et al.* [22]. For CO_2 rich mixtures the experiments from Botros *et al.* [23] has been sourced.

All the experiments sourced have similar set-up and many things in common. The experiments are performed in a horizontal shock-tube comprised of a number of tubular sections flanged together and equipped with pressure and temperature transducers located along the length of the shock-tube. One end is closed and the other end is equipped with a rupture disc. In order to ensure controllable and uniform temperature the shock-tube is heat traced and insulated. The facilities has mixing and compression units in order to fill the shock tube with the desired mixture and the desired initial pressure. For additional information about experimental methods and facility description and details please refer to the original papers [21, 22].

The experimental test conditions for the pure CO_2 experiments are summarised in Table 1 and the experimental test conditions for the CO_2 rich mixtures are summarised in Table 2.

Exp No.	P (bar)	T (°C)	Source
3	40.4	10.2	Munkejord et al.
6	104	40	Munkejord et al.
8	122.2	24.6	Munkejord et al.
15	340.4	36.5	Botros et al.
31	111.11	35.04	Botros et al.
32A	112.7	8.74	Botros et al.

Table 1: Experimental initial conditions for decompression experiments with pure CO_2 from Munkejord *et al.* [21] and Botros *et al.* [22].

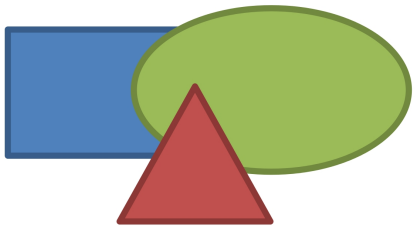

Figure 1: Each figure and table caption is put below the figure and typeset like this caption. Compose good, comprehensive captions.

			Composition (mole %)							
Exp No.	**Pressure (bar)**	**Temperature (°C)**	**CO_2**	**N_2**	**O_2**	**He**	**Ar**	**CO**	**H_2**	**CH_4**
2	148.3	35.9	94.03	5.82	0.127	0.025				
4	145.6	35.1	96.67		3.33					
7	147.8	36.3	96.52			0.0138				3.47
10B	149.3	35.3	96.77						3.23	
5	144.9	35.6	96.77	0.0025				3.23		
9	154.6	35.2	96.14				3.86			

Table 2: Experimental initial conditions for decompression experiments with pure CO_2 from Botros *et al.* [23].

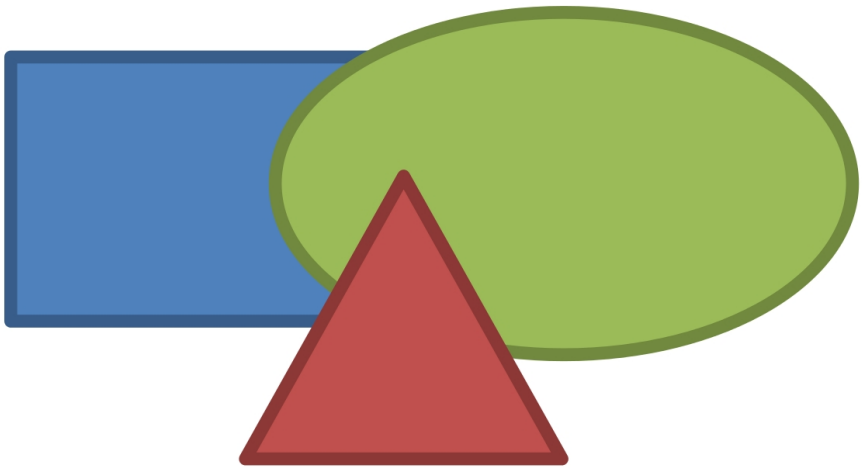

Figure 2: A two-column spanning figure.

2 Results and discussion

2.1 Pure CO_2

2.2 CO_2 mixtures

Acknowledgement

Acknowledgements come here.

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Appendix

If there is the need for an appendix, this is the right place for it. Again use an unumbered section for this purpose, as already used for the introduction.