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:

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

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].

2 Results and discussion

2.1 Pure CO_2

The experiments for pure CO_2 summarised in Table 1 have all been simulated using the Span & Wagner equation of state as provided by CoolProp. The isentropic decompression path for all simulated cases is shown in Figure 1.The path from the inital pressure and temperature in the single phase region to the saturation line. The experimental initial conditions cover both gas, liquid (supercritical), and supercritical fluid. Once the decompression state reaches the saturation line the isentrope follows the saturation line with varying fase split. Calculations have been done with the REFPROP backend as well, and identical results where obtained (not shown).

Exp No.	Pressure (bar)	Temperature (°C)	Composition (mole %)							
			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].
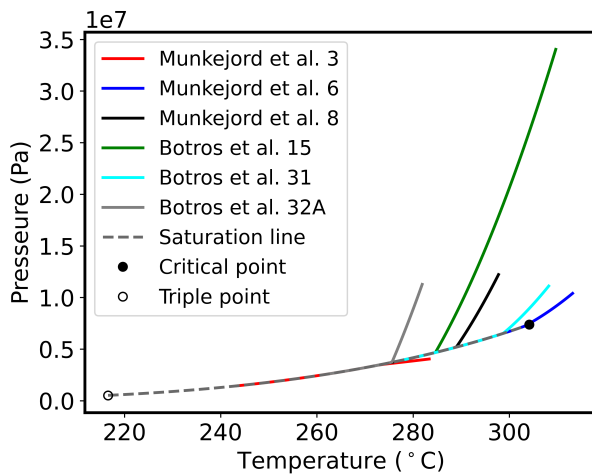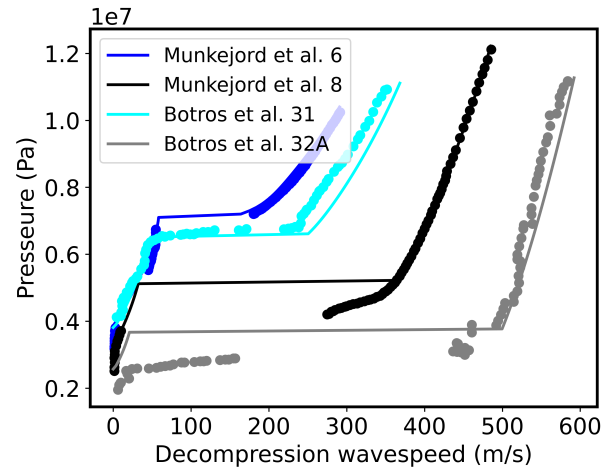

Figure 1: Isentropic decompresion path for all simulated cases for pure CO_2 shown in the P,T plane along with the saturation curve for pure CO_2 from triple point to the critical point.

Decompression wave speed plots are made for all cases and corresponding experimental data has been sourced from [21, 22]. It shall be noted that the experimental points have been read manually with the aid of the ScanIT program from Amsterchem [1]. Some slight inaccuracy during the digitization of data from the original references must be expected and further in some areas the original data was too dense to allow all data points to be extracted. That being said the overall characteristics and the shape of the decompression curves have been retained.

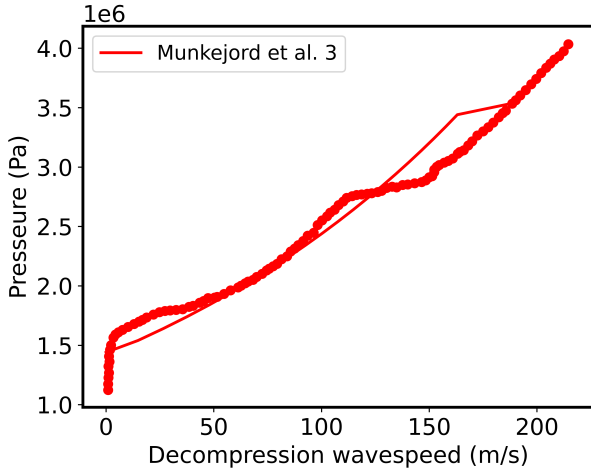The decompression curves for experiments 6 and 8 from [21] and experiments 31 and 32A from [22] are

grouped in the same plot cf. Figure 2 whereas experiments 3 from [21] and 15 from [22] are plotted individually in Figures 3 and 4 , respectively.
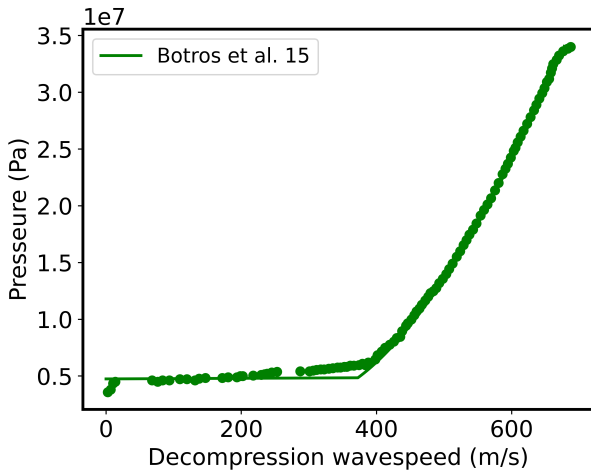

Figure 2: Decompression curves for pure CO_2 calculated with the RAMDECOM code and experimental data.

Generally the following observations are made: First of all, the isentropic decompression path follows a gradual decrease in decompression wave speed as the pressure is reduced. Once the saturation line / two-phase state is reached the decompression wave speed abrubtly drops due to an abrupt drop in the speed of sound, which is seen as a plateau in the pressure. Second, it seems that the described decompression wave speed model matches experiments very well for decompression from a supercritical fluid state and this applies to experiments no. 6 [21], 15 [22] and 31 [22] as seen from Figure 2 and 4. Especially the plateau pressure as described previously, is predicted vary well for these cases. Finally, the cases where the decompression starts

Figure 3: Decompression curve for pure CO_2 calculated with the RAMDECOM code and data for experiment 3 from [21].

Figure 4: Decompression curve for pure CO_2 calculated with the RAMDECOM code and data for experiment 15 from [22].

in the supercritical liquid state and in the gas state are predicted less accurately. This applies to experiments no. 8 [21], 32A [22] cf. Figure 2 and to some extent experiment no. 3 [21] cf. Figure 3.

In case of experiment no. 3 in Figure 3 the model predicts a slight pressure plateau at around 3.5 MPa, which is where the theoretical isentropic path intersects the saturation line. However, the experimental data shows a plateau around 2.8 MPa somewhat lower. Munkejord *et al.* [21] demonstrated that the experimen-

tal data was reasoanbly described is a single phase isentropic path was followed all the way from the initial pressure to the experimental plateau, also supporting a hypothesis that full equilibrium is not established instantaneously and a significant sub-cooling of the gas phase occurs before the first liquid droplets starts to form.

Experiments 8 and 32A are very similar and in both cases the discrepancy between the predicted plateau pressure and the experimental data have been rationalised by both Botros *et al.* [22] and Munkejord *et al.* [21] by a very rapid decompression, since the initial pressure is not far from the saturation pressure, in which equilibrium is not due to delayed nucleation. This leads to a measured plateau below the predicted. In both this case and the one for experiment 3 starting from the gas phase it is evident that any non-equilibrium effects be it delayed nucleation or sub-cooled gas, leads to a conservative result from the simple decompression model.

2.2 CO_2 mixtures

The calculated decompression curves for the CO_2 mixtures in Table 2 are shown in Figure 5 along with the corresponding experimental data from [23]. As seen from the figure experiments no. 4, no. 5, no. 7, and no. 9 are predicted very well by the simple decompression model. The repdictions for these experiments are generally in line with both predictions like the one in the present study using the GERG-2008 [23] equation of state as well as predictions made with GASDECOM [1].

The main discrepancies between model and experiment are observed for experiment no. 2 and no. 10B, In both cases the simple decompression model underpredicts the plateau pressure. For 10B, which contains a significant amount of hydrogen in a binary mixture, the same model behaviour is observed by Botros *emph* [23]. As observed for the pure CO_2 the failure to produce equilibriunm conditions during experiments generally resulted in an over-prediction of the experimentally observed plateau. The fact that the plateau is under-predicted for the H_2/CO_2 binary mixture could indicate that this is due to a defficiency in the applied equation of state to accurately model the bubble point line in particular. This should be investigated in more detail in future works.

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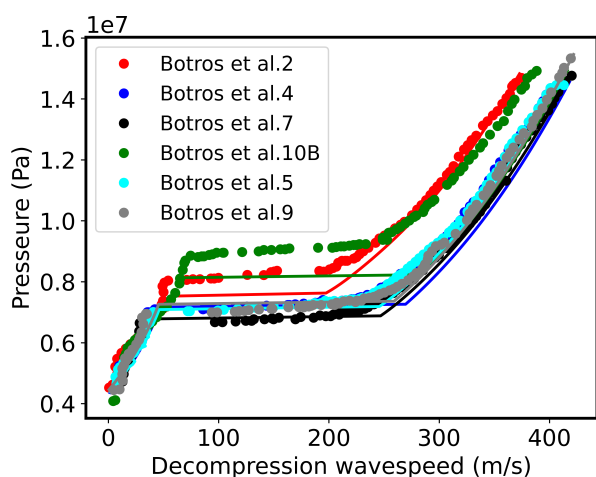
Figure 5: Decompression curves for rich CO$_2$ mixtures calculated with the RAMDECOM code and experimental data from [23].

Acknowledgement

Acknowledgements come here.

References

[1] Andrew Cosham, Robert J. Eiber, and Edward B. Clark. GASDECOM: Carbon Dioxide and Other Components. volume 2 of *2010 8th International Pipeline Conference*, pages 777–794, 09 2010.

[2] C. Lu, G. Michal, A. Elshahomi, A. Godbole, P. Venton, K. K. Botros, L. Fletcher, and B. Rothwell. Investigation of the effects of pipe wall roughness and pipe diameter on the decompression wave speed in natural gas pipelines. *Proceedings of the Biennial International Pipeline Conference, IPC*, 3:315–322, 2012.

[3] Andrew Cosham, David G. Jones, Keith Armstrong, Daniel Allason, and Julian Barnett. The Decompression Behaviour of Carbon Dioxide in the Dense Phase. volume 3: Materials and Joining of *International Pipeline Conference*, pages 447–464, 09 2012.

[4] Bin Liu, Xiong Liu, Cheng Lu, Ajit Godbole, Guillaume Michal, and Anh Kiet Tieu. Multiphase decompression modeling of co2 pipelines. *Greenhouse Gases: Science and Technology*, 7(4):665–679, 2017.

[5] B. P. Xu, H. E. Jie, and J. X. Wen. A pipeline depressurization model for fast decompression and slow blowdown. *International Journal of Pressure Vessels and Piping*, 123-124:60–69, nov 2014.

[6] Adeyemi Oke, Haroun Mahgerefteh, Ioannis Economou, and Yuri Rykov. A transient outflow model for pipeline puncture. *Chemical Engineering Science*, 58(20):4591–4604, 2003.

[7] Alhoush Elshahomi, Cheng Lu, Guillaume Michal, Xiong Liu, Ajit Godbole, and Philip Venton. Decompression wave speed in co2 mixtures: Cfd modelling with the gerg-2008 equation of state. *Applied Energy*, 140:20–32, 2015.

[8] Shuaiwei Gu, Yuxing Li, Lin Teng, Qihui Hu, Datong Zhang, Xiao Ye, Cailin Wang, Jinghan Wang, and Stefan Iglauer. A new model for predicting the decompression behavior of CO$_2$ mixtures in various phases. *Process Safety and Environmental Protection*, 120:237–247, 2018.

[9] Qihui Hu, Nan Zhang, Yuxing Li, Wuchang Wang, Jianlu Zhu, and Jiyu Gong. A new model for calculation of arrest toughness in the fracture process of the supercritical CO$_2$ pipeline. *ACS Omega*, 6(26):16804–16815, 2021. PMID: 34250340.

[10] Ian H. Bell, Jorrit Wronski, Sylvain Quoilin, and Vincent Lemort. Pure and pseudo-pure fluid thermophysical property evaluation and the open-source thermophysical property library coolprop. *Industrial & Engineering Chemistry Research*, 53(6):2498–2508, 2014.

[11] E W Lemmon, I H Bell, M L Huber, and M O McLinden. NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 10.0, National Institute of Standards and Technology, 2018.

[12] R. Span and W. Wagner. A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple-Point Temperature to 1100 K at Pressures up to 800 MPa. *Journal of Physical and Chemical Reference Data*, 25(6):1509, oct 2009.

[13] E. W. Lemmon and R. T. Jacobsen. A Generalized Model for the Thermodynamic Properties of Mixtures. *International Journal of Thermophysics 1999 20:3*, 20(3):825–835, 1999.

[14] O. Kunz and W. Wagner. The GERG-2008 Wide-Range Equation of State for Natural Gases and Other Mixtures: An Expansion of GERG-2004. *Journal of Chemical and Engineering Data*, 57(11):3032–3091, nov 2012.

[15] Johannes Gernert and Roland Span. EOS–CG: A Helmholtz energy mixture model for humid gases and CCS mixtures. *The Journal of Chemical Thermodynamics*, 93:274–293, feb 2016.

[16] Stefan Herrig. *New Helmholtz-Energy Equations of State for Pure Fluids and CCS-Relevant Mixtures*. PhD thesis, Ruhr Universität Bochum, Bochum, 2018.

[17] Anders Andreasen. HydDown: A Python package for calculation of hydrogen (or other gas) pressure vessel filling and discharge. *Journal of Open Source Software*, 6(66):3695, oct 2021.

[18] Wes McKinney. Data structures for statistical computing in python. In Stéfan van der Walt and Jarrod Millman, editors, *Proceedings of the 9th Python in Science Conference*, pages 51 – 56, 2010.

[19] J. D. Hunter. Matplotlib: A 2d graphics environment. *Computing In Science & Engineering*, 9(3):90–95, 2007.

[20] Charles R. Harris, K. Jarrod Millman, St'efan J. van der Walt, Ralf Gommers, Pauli Virtanen, David Cournapeau, Eric Wieser, Julian Taylor, Sebastian Berg, Nathaniel J. Smith, Robert Kern, Matti Picus, Stephan Hoyer, Marten H. van Kerkwijk, Matthew Brett, Allan Haldane, Jaime Fern'andez del R'ıo, Mark Wiebe, Pearu Peterson, Pierre G'erard-Marchant, Kevin Sheppard, Tyler Reddy, Warren Weckesser, Hameer Abbasi, Christoph Gohlke, and Travis E. Oliphant. Array programming with NumPy. *Nature*, 585(7825):357–362, 2020.

[21] Svend Tollak Munkejord, Anders Austegard, Han Deng, Morten Hammer, H.G. Jacob Stang, and Sigurd W. Løvseth. Depressurization of CO_2 in a pipe: High-resolution pressure and temperature data and comparison with model predictions. *Energy*, 211:118560, 2020.

[22] K. K. Botros, J. Geerligs, B. Rothwell, and T. Robinson. Measurements of Decompression Wave Speed in Pure Carbon Dioxide and Comparison With Predictions by Equation of State. *Journal of Pressure Vessel Technology*, 138(3), 12 2015. 031302.

[23] K. K. Botros, J. Geerligs, B. Rothwell, and T. Robinson. Measurements of Decompression Wave Speed in Binary Mixtures of Carbon Dioxide and Impurities. *Journal of Pressure Vessel Technology*, 139(2), 09 2016. 021301.

Appendix

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