Central European Journal of Energetic Materials
ISSN 1733-7178; e-ISSN 2353-1843

Cent. Eur. J. Energ. Mater. 2023, *20*(1): 5-13; DOI 10.22211/cejem/162850
Article is available in PDF-format, in colour, at:
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Research paper

Comparison of the Implemented Detonation Velocity Predictions in the Research Output Software for Energetic Materials Based on Observational Modelling (RoseBoom©) with 30 Experimental Values

Sabrina Wahler[1,2,*)], **Thomas M. Klapötke**[1,**)]

[1)] *Department of Chemistry, Energetic Materials Research, Ludwig-Maximilian University of Munich, 81377 Munich, Germany*

[2)] *RoseExplosive UG (haftungsbeschränkt), Munich, Germany*

E-mails: *) sabrina.wahler@roseexplosive.com;
,) tmk@cup.uni-muenchen.de

ORCID information:

Wahler S.: https://orcid.org/0000-0002-7515-0148
Klapötke T.M.: https://orcid.org/0000-0003-3276-1157

Abstract: So far, the accuracy of the new Computer Software RoseBoom© has only been determined by comparing it to the Program EXPLO5. In the present study RoseBoom©'s predictions are compared with 30 experimental detonation velocities, in order to evaluate which of the computer codes is more accurate.

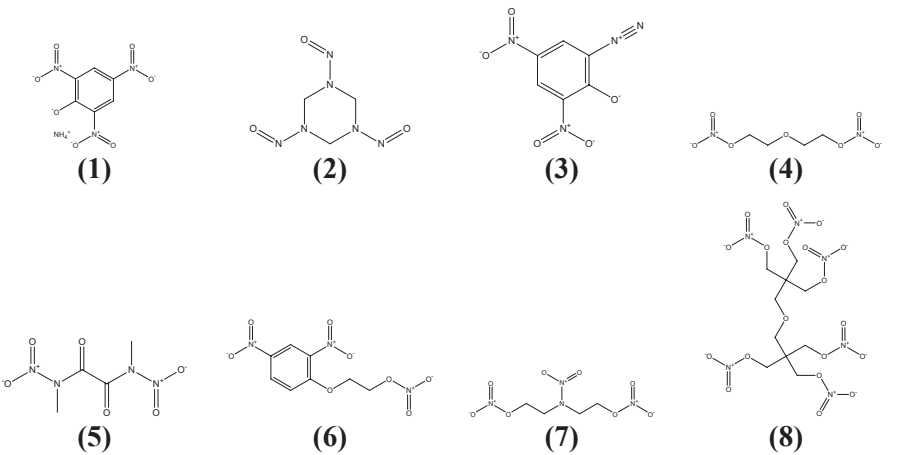
Keywords: experimental values, computer software, prediction, RoseBoom, detonation velocity

1 Introduction

Current computer programs like EMDB or EXPLO5 for energetic materials all require the time consuming manual input of the sum formula, density and heat of formation [1, 2]. The necessary heat of formation and density require a prior synthesis or time-consuming composite methods. Recent advances directly addressing this problem and overcoming it were made with the Software RoseBoom2.1© (Research output software for energetic materials based on observational modelling) [3]. This Software combines empirical relationships for energetic materials published in different epochs of high-energy density materials (HEDMs) research. These have been revalidated for modern compounds on a dataset of over 480 pure compounds [4, 5] and 518 energetic mixtures calculated in EXPLO5 [6] and merged in the user-friendly tool RoseBoom©, which allows quick and easy access to the performance parameters of HEDMs [5]. The RoseBoom© program has only been validated on EXPLO5 values due to the lack of experimental values, because a large dataset was desirable to quickly assess whether the selected models give reliable results. This new study is focused on revalidating them against experimental detonation velocities measured under confinement. This is done on a dataset of thirtyone selected molecules, the detonation velocities (VODs) of which were measured under confinement.

2 Results and Discussion

Structural formulae of the analyzed substances are presented in Figure 1. The results are displayed in Figure 2 and Table 1.



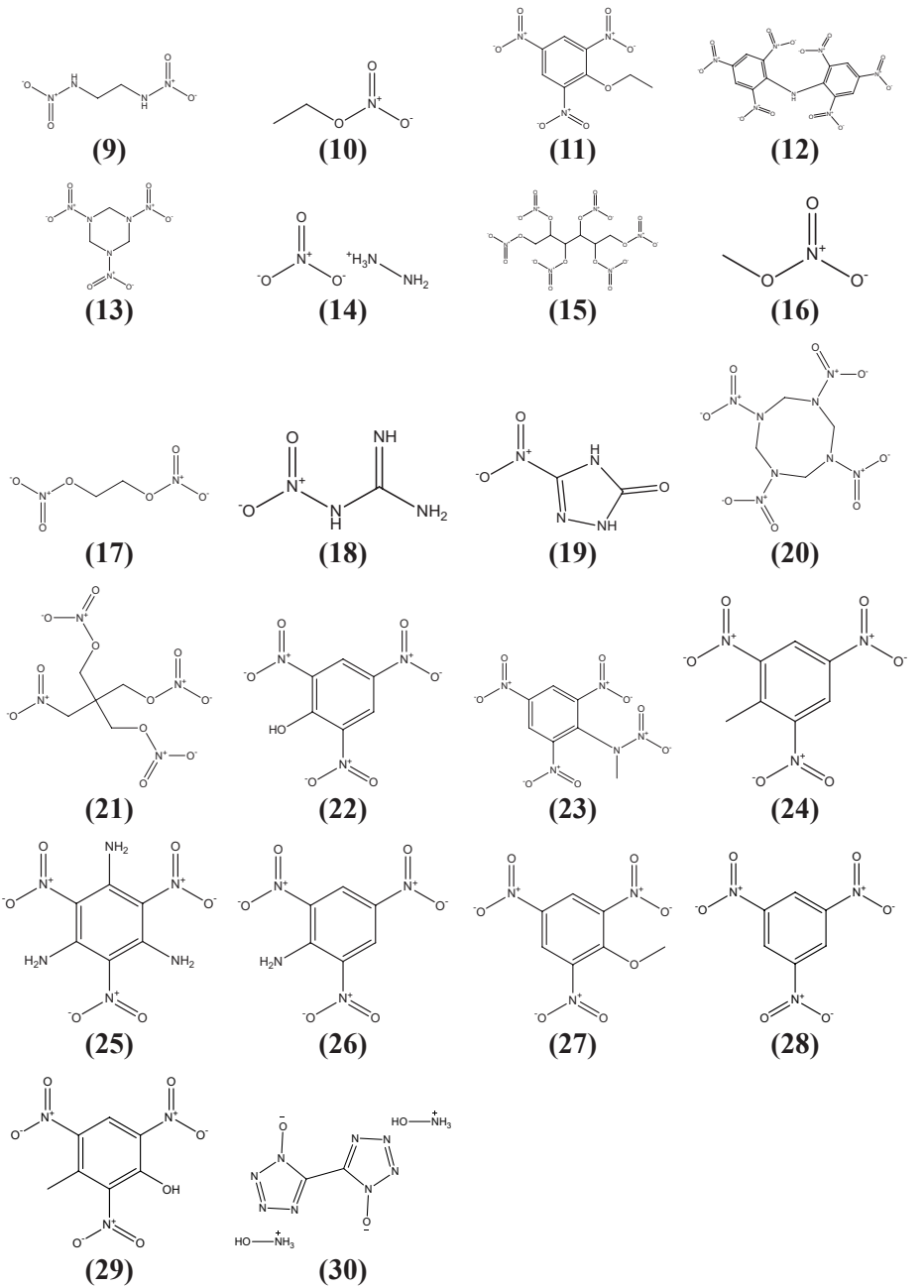


Figure 1. Structural formulae of the 30 substances analyzed in RoseBoom2.2©

Table 1. Dataset of molecules calculated in RoseBoom2.2© with the corresponding experimental VODs under confinement, plus the packing densities and heats of formation used in the calculations

Formula	VOD [m/s] and (deviation from experimental value [%])							Packing density [g/cm^3] [7]	Heat of formation [kJ/mol] [7]
	Experimental (confined) [7]	Keshavarz [8]	Rothstein and Petersen [9]	Kamlet and Jacobs [10]	Stine [11]	RoseHybrid	EXPLO5 V6.05.04 (BKW EOS, BKWN (default))		
(1)	7150 (–)	7396 (3.4)	7397 (3.5)	6957 (2.7)	6969 (2.5)	7180 (0.4)	6766 (5.4)	1.6	–386.5
(2)	7300 (–)	7261 (0.5)	7880 (7.9)	7361 (0.8)	7628 (4.5)	7532 (3.2)	7568 (3.7)	1.49	285.8
(3)	6600 (–)	6915 (4.8)	7214 (9.3)	6697 (1.5)	6891 (4.4)	6929 (5.0)	6874 (4.2)	1.5	194.1
(4)	6600 (–)	6839 (3.6)	6507 (1.4)	7022 (6.4)	6900 (4.5)	6817 (3.3)	6908 (4.7)	1.38	–436.8
(5)	7100 (–)	7222 (1.7)	7201 (1.4)	6999 (1.4)	7118 (0.3)	7135 (0.5)	6873 (3.2)	1.48	–305.5
(6)	6800 (–)	7018 (3.2)	6314 (7.1)	6895 (1.4)	6736 (0.9)	6741 (0.9)	6658 (2.1)	1.58	–292.9
(7)	7580 (–)	7342 (3.1)	7553 (0.4)	7577 (0.0)	7525 (0.7)	7499 (1.1)	7435 (1.9)	1.47	–275.7
(8)	7400 (–)	7850 (6.1)	7115 (3.9)	7862 (6.2)	7632 (3.1)	7615 (2.9)	7565 (2.2)	1.6	–928.5
(9)	7570 (–)	7507 (0.8)	8309 (9.8)	8087 (6.8)	8112 (7.2)	8004 (5.7)	8213 (8.5)	1.65	–103.8
(10)	5800 (–)	5813 (0.2)	4951 (14.6)	6050 (4.3)	6138 (5.8)	5738 (1.1)	6152 (6.1)	1.1	–190.4

Table 1. Continuation

Formula	VOD [m/s] and (deviation from experimental value [%])							Packing density [g/cm^3] [7]	Heat of formation [kJ/mol] [7]
	Experimental (confined) [7]	Keshavarz [8]	Rothstein and Petersen [9]	Kamlet and Jacobs [10]	Stine [11]	RoseHybrid	EXPLO5 V6.05.04 (BKW EOS, BKWN (default))		
(11)	6500 (–)	6832 (5.1)	6303 (3.0)	6672 (2.6)	6545 (0.7)	6588 (1.4)	6423 (1.2)	1.55	–200.8
(12)	7200 (–)	7111 (1.2)	7444 (3.4)	7081 (1.7)	7121 (1.1)	7189 (0.2)	7038 (2.3)	1.6	41.4
(13)	8750 (–)	8524 (2.6)	8940 (2.2)	8655 (1.1)	8669 (0.9)	8697 (0.6)	8648 (1.2)	1.76	66.9
(14)	8690 (–)	7544 (13.2)	8479 (2.4)	8383 (3.5)	8678 (0.1)	8271 (4.8)	8364 (3.8)	1.6	–247.9
(15)	8260 (–)	9043 (9.5)	7543 (8.7)	8776 (6.2)	8623 (4.4)	8496 (2.9)	8166 (1.1)	1.73	–675.7
(16)	6100 (–)	6614 (8.4)	5836 (4.3)	6096 (0.1)	6105 (0.1)	6163 (1.0)	8020 (31.5)	1.47	–27.2
(17)	7300 (–)	7454 (2.1)	7618 (4.4)	7972 (9.2)	7896 (8.2)	7735 (6.0)	7478 (2.4)	1.48	–242.8
(18)	8200 (–)	7711 (6.0)	8262 (0.8)	7650 (6.7)	8188 (0.1)	7953 (3.0)	8343 (1.7)	1.71	–92.9
(19)	7940 (–)	7843 (1.2)	8753 (10.2)	7629 (3.9)	8029 (1.1)	8064 (1.6)	7831 (1.4)	1.77	–100.7
(20)	9100 (–)	9172 (0.8)	9042 (0.6)	8924 (1.9)	8890 (2.3)	9007 (1.0)	9030 (0.8)	1.9	–75
(21)	8400 (–)	8295 (1.3)	7575 (9.8)	8322 (0.9)	8096 (3.6)	8072 (3.9)	8017 (4.6)	1.7	–511.5

Table 1. Continuation

Formula	VOD [m/s] and (deviation from experimental value [%])							Packing density [g/cm^3] [7]	Heat of formation [kJ/mol] [7]
	Experimental (confined) [7]	Keshavarz [8]	Rothstein and Petersen [9]	Kamlet and Jacobs [10]	Stine [11]	RoseHybrid	EXPLO5 V6.05.04 (BKW EOS, BKWN (default))		
(22)	7350 (–)	7703 (4.8)	7359 (0.1)	7320 (0.4)	7234 (1.6)	7404 (0.7)	7162 (2.6)	1.7	–248.5
(23)	7570 (–)	7752 (2.4)	7772 (2.7)	7713 (1.9)	7619 (0.6)	7714 (1.9)	7599 (0.4)	1.71	20
(24)	6900 (–)	7084 (2.7)	6665 (3.4)	6856 (0.6)	6744 (2.3)	6837 (0.9)	6634 (3.9)	1.6	–67.1
(25)	7350 (–)	7307 (0.6)	7861 (7.0)	7956 (8.2)	7865 (7.0)	7747 (5.4)	7994 (8.8)	1.8	139.7
(26)	7300 (–)	7470 (2.3)	7497 (2.7)	7367 (0.9)	7297 (0.0)	7408 (1.5)	7242 (0.8)	1.72	–84
(27)	6800 (–)	7080 (4.1)	6800 (0.0)	6926 (1.9)	6838 (0.6)	6911 (1.6)	6804 (0.1)	1.57	–153.2
(28)	7300 (–)	7637 (4.6)	7277 (0.3)	7109 (2.6)	7035 (3.6)	7264 (0.5)	6930 (5.1)	1.71	–204.2
(29)	6850 (–)	7242 (5.7)	6800 (0.7)	6938 (1.3)	6829 (0.3)	6952 (1.5)	6685 (2.4)	1.62	–252.4
(30)**)	8870 (–)	8551 (3.6)	9791 (10.4)	8358 (5.8)	8790 (0.9)	8872 (0.0)	8987 (1.3)	1.748	213.4

**) – Ref. [12]

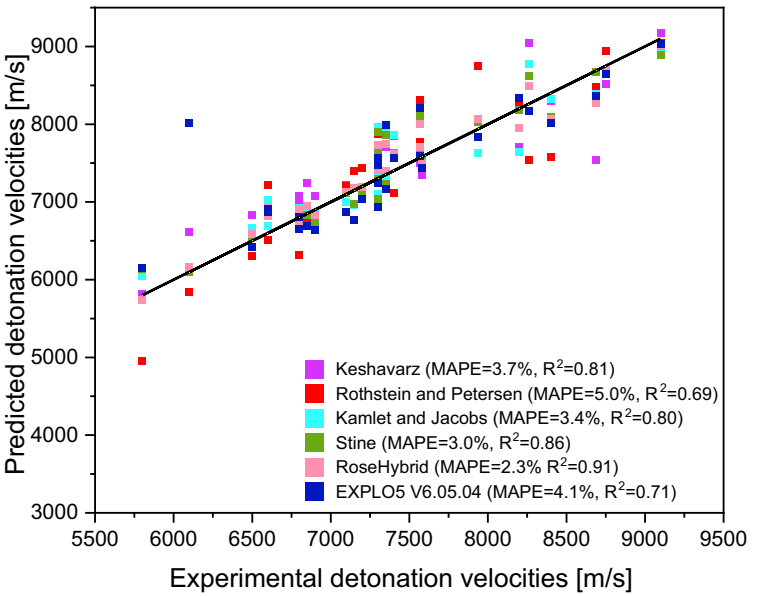


Figure 2. Experimental detonation velocities under confinement compared to the predictions in RoseBoom©

When comparing RoseBoom©'s detonation velocities to the EXPLO5 velocities, which deviate by 5% from experimental values [1], it was not clear if the deviations of RoseBoom's values were closer to the experimental values than those from EXPLO5 or even further away. The results given in Figure 2 prove that the EXPLO5 values deviate by 4.9% from the literature values, which is within the range of the reported deviations [1], but it was also discovered that the coefficient of determination was low with $R^2 = 0.71$. Additionally, a new ground-breaking discovery made in this study is that all of the empirical modelling approaches outperformed the thermo equilibrium code EXPLO5, because either the mean absolute percentage error was lower, the R^2-coefficient was higher or both. Surprisingly, the errors in the individual empirical approaches obliterate each other, staying within 2.3% of the experimental values. This slight scattering might also be caused by measurement errors in the collected literature values [12]. The errors can have various causes, like inhomogeneous packing, hydratisation of the compounds or impurities, along with many other possibilities. It can be assumed that the RoseHybrid©-values are closer to the experimental values than the other methods individually or the EXPLO5 values, because more features are taken into consideration. These features range from the functional groups present, considered in the Keshavarz model and the Rothstein and Petersen

method, along with the oxygen balance, considered in the Stine Method and the detonation products considered in the Kamlet and Jacobs method.

3 Conclusions

- As a conclusion, one can say that thermo-equilibrium codes can be replaced by the program RoseBoom©, which gives results closer to the experimental detonation velocities.
- It is not possible to make predictions that are more accurate than the experiment values, which is why more precise experimental data on the measurement of detonation parameters is needed. Until experimental scientists can provide the necessary data, the RoseHybrid©-value is as close as it can be to the experimental value, because these predictions lie within experimental uncertainties.

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Received: October 25, 2022
Revised: March 30, 2023
First published online: March 31, 2023
Updated: April 12, 2023