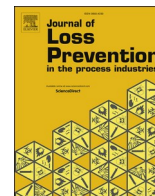




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Prediction of BLEVE mechanical energy by implementation of artificial neural network

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ABSTRACT

In the event of a BLEVE, the overpressure wave can cause important effects over a certain area. Several thermodynamic assumptions have been proposed as the basis for developing methodologies to predict both the mechanical energy associated to such a wave and the peak overpressure. According to a recent comparative analysis, methods based on real gas behavior and adiabatic irreversible expansion assumptions can give a good estimation of this energy. In this communication, the Artificial Neural Network (ANN) approach has been implemented to predict the BLEVE mechanical energy for the case of propane and butane. Temperature and vessel filling degree at failure have been considered as input parameters (plus vessel volume), and the BLEVE blast energy has been estimated as output data by the ANN model. A Bayesian Regularization algorithm was chosen as the three-layer backpropagation training algorithm. Based on the neurons optimization process, the number of neurons at the hidden layer was five in the case of propane and four in the case of butane. The transfer function applied in this layer was a sigmoid, because it had an easy and straightforward differentiation for using in the backpropagation algorithm. For the output layer, the number of neurons had to be one in both cases, and the transfer function was *purelin* (linear). The model performance has been compared with experimental values, proving that the mechanical energy of a BLEVE explosion can be adequately predicted with the Artificial Neural Network approach.

1. Introduction

BLEVEs are strong explosions associated to the catastrophic failure of a vessel containing a liquid plus vapor at a temperature significantly higher than its boiling temperature at atmospheric pressure; the instantaneous increase in volume of both liquid and vapor generates an overpressure wave which can be very strong. This wave can be attributed to the liquid vaporization or to the expansion of the pre-existent vapor, and this can lead to different values. Another possibility is to assume the added effect of both phenomena, this later approach being the most conservative.

In order to calculate this overpressure and its effects and consequences, the mechanical energy associated to it must be known.

Several methods to calculate BLEVE mechanical energy have been proposed, which are based on different thermodynamic assumptions:

- constant volume energy addition (Brode, 1959)
- ideal gas behavior and isentropic expansion (Prugh, 1991)
- thermodynamic availability (Crowl, 1991, 1992)
- isothermal expansion (Smith et al., 1996)
- real gas behavior and adiabatic irreversible expansion (Planas-Cuchi et al., 2004)
- real gas behavior and isentropic expansion (CCPS, 2010).

These methods take into account the contribution of both the liquid vaporization and the pre-existing vapor expansion. Furthermore, another approach has been proposed (Casal and Salla, 2006, based on the superheating energy SE) which takes into account only the vaporization of the liquid. According to a comparative analysis (Hemmatian et al., 2017a), the methods based on the assumptions of ideal gas behavior and isentropic expansion give rather conservative results,

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while the methods based on real gas behavior and adiabatic irreversible expansion give more realistic values. Following a relatively different approach (Hemmatian et al., 2017b), the mechanical energy can be estimated as a function of the vessel filling degree and temperature at the rupture moment. In practice, however, it should be taken into account that only part of the mechanical energy is invested in creating the overpressure. The other part is used for breaking the vessel and fragmentation. In the case of ductile failure, approximately 40% of the mechanical energy is converted to blast. However, this number could vary between 40% and 50% depending on the circumstances.

From the point of view of the emergency management, a BLEVE can occur at any moment depending on the circumstances when a vessel is under the effects of fire (Hemmatian et al., 2015). For example, the first BLEVE in San Juanico accident (1984) happened after 69 s of the first explosion (which probably originated several jet fires). However, the time to failure can be more prolonged: for example, it has been reported that an LPG tanker BLEVED after 70 min of being exposed to fire (Planas et al., 2015). Anyway, the prediction of BLEVE mechanical energy is quite important to define the possible effects and the safe distances.

Some of the existing methods require complex thermodynamic information and calculations. A different approach that can help in solving this problem could be that based on the Artificial Neural Network (ANN), used nowadays as a handy toolkit for the simulation, prediction and modeling of various engineering and scientific problems.

In this study, the ANN approach has been implemented to produce a function for calculating the BLEVE mechanical energy, specifically for propane and butane as the most common substances involved in BLEVE accidents (Hemmatian et al., 2019). The function thus obtained only depends on the rupture temperature and vessel filling level. The values thus obtained have been compared with some experimental data taken from the literature.

2. Theory and methods

2.1. Dataset preparation

Two datasets for propane and butane were prepared for the ANN approach by using a method based on real gas behavior and adiabatic irreversible expansion (Planas-Cuchi et al., 2004). The required thermodynamic data were obtained from NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP) version 9.1. (Lemmon et al., 2007). Temperature (K), filling level (%) and mechanical energy (MJ/m³) were registered in the datasets. The database interval was designed for filling level ranging between 1% and 90% in the case of propane, and between 1% and 99% for butane. The initial temperatures were 300 K and 283 K for both propane and butane. The ANN was trained in those aforementioned intervals. Propane and butane datasets had 121 and 201 data points, respectively. Those datasets were used in the ANN for generating the related functions. Finally, the resulting functions were applied to two sets of experimental data to analyze the goodness of the method.

2.2. BLEVE experimental data

Two sets of experimental data were used to check the models' performances. In Johnson experiments (Johnson et al., 1990; Laboureur et al., 2014), there are 7 BLEVE data obtained by using butane and propane (Table 1). The contained liquid was heated with electric immersion. The vessels were ruptured by the detonation of a linear explosive. The overpressure was measured at 25, 50, 100 and 150 meters away.

9 fired propane BLEVE experiments were reported by Birk et al. (Birk and VanderSteen, 2006; Birk et al., 2007). The overpressure was measured at 10, 20, 30 and 40 meters away (Table 2).

Table 1

Johnson experiments (Johnson et al., 1990; Laboureur et al., 2014).

Johnson	Fluid	m(kg)	V(m ³)	P _{rupt} (kPa)	Filling Level (%)
1	Butane	2000	5.659	1460	75
2	Butane	2000	5.659	1510	76
3	Butane	1000	5.659	1520	38
4	Butane	2000	5.659	770	68
5	Butane	2000	10.796	1510	40
6	Propane	2000	5.659	1520	77
7	Butane	2000	5.659	1520	76

2.3. Artificial neural network (ANN)

Neurons are the basic elements of the biological neural network in the human brain. A neuron receives data from neighboring neural cells through dendrites and makes some process in the soma (body), transferring a signal to the next neuron through the axon; data transfer is performed by synapses through electrochemical signals (Yadav et al., 2014).

The Artificial Neural Networks can be applied to analyze and calculate data for different problems and solve them with the same pattern as that of a biological neural network. The first attempts in this field were due to Hebb in the 1940s (Hebb, 1949). After that, some researchers such as Hopfield, Rumelhart, Grossberg and Widrow developed this method in the 1980s (Hopfield, 1982; Rumelhart et al., 1986; Grossberg, 1982; Widrow et al., 1987).

With ANN, complicated problems could be solved through parallel and distributed processing. It solves problems without requiring too complicated formulation; because of this, it could save time significantly in comparison with closed-form solving methods. Moreover, this methodology enables to approximate any non-linear function to a compact set of data with a specified accuracy (Siddique and Adeli, 2013).

Every neuron model consists of a segment that signals (i.e., input variables) import through it and acts like a synapse. At first, each one of the inputs (x_i) is multiplied by its corresponding weight value " w ". After the summation of these values, a bias value " b " can be added to the result. A summary of this process for n inputs is shown in Eq. (1):

$$net = \left(\sum_{i=1}^n w_i x_i \right) + b \quad (1)$$

At the end of this process, the result enters in a transfer function (i.e., f) and gives output values (i.e., y), Eq. (2):

$$y = f(net) \quad (2)$$

The usual forms of the transfer function are linear, step, ramp or sigmoid. Fig. 1 shows the structure of an ANN.

Some neurons connect, forming a layer of neurons. A network includes one or more of these layers. According to the configuration and the way of connection between neurons, there can be different types of neural networks. Generally, they can be separated into two categories: 1) feedforward neural networks, and 2) feedback neural networks.

In a feedforward neural network, the signals travel in a forward way,

Table 2

Birk experiments (Birk and VanderSteen, 2006; Birk et al., 2007).

Birk	Fluid	m (kg)	V(m ³)	P _{rupt} (kPa)	Filling Level (%)
1	Propane	150	2	1863	17
2	Propane	309.3	2	1846	35
3	Propane	117	2	1699	13
4	Propane	184.6	2	1894	21
5	Propane	116.9	2	1573	12
6	Propane	453.1	2	1803	51
7	Propane	475.1	2	1563	52
8	Propane	470.3	2	1813	53
9	Propane	538.4	2	1858	61

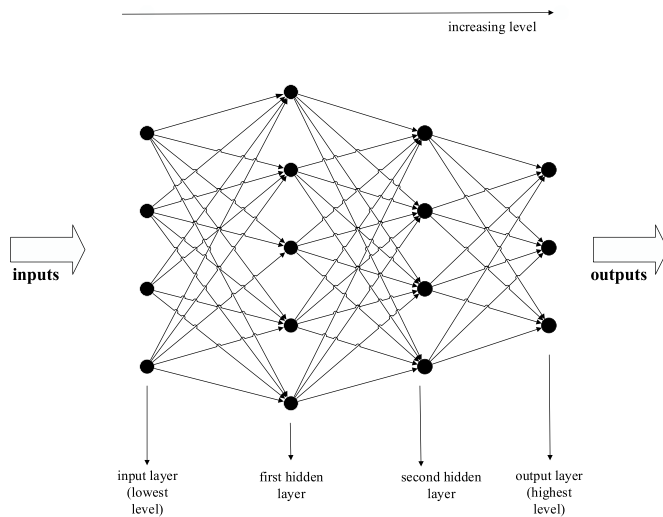


Fig. 1. Structure of an artificial neural network (Siddique and Adeli, 2013).

they cannot come back, and there is no feedback. This type of neural network (e.g., Fig. 2) can be represented in vector form by Eq. (3):

$$Y = f(W \cdot x + b) \quad (3)$$

Here, Y is the output vector, W is the weight matrix, b is a bias vector and f is a transfer function.

The primary task of the neural network is to define the weights and biases in a way that adapts the output to the inputs with a minimum error. A training process does the modification of weights and biases. The training method used for solving the network in this work has been the Bayesian Regulation one, which can be applied to feedforward neural networks training. It is based on a statistical approach and assumes that the values of weights and biases are related to a distribution function with unknown variance. The primary task is to estimate the parameters using statistical techniques (Siddique and Adeli, 2013; Foresee and Hagan, 1997; Nguyen, 1998).

3. Results and discussion

3.1. Backpropagation training algorithm

Three different backpropagation (BP) algorithms, i.e., Levenberg – Marquardt (Hagan and Menhaj, 1994), Bayesian Regularization (MacKay, 1992; Ticknor, 2013) and Scaled Conjugate Gradient (Möller, 1993), were studied to find the best one for the ANN. Five neurons were considered for the comparative study and, finally, the algorithm with the lowest mean square error (MSE) was chosen as the BP algorithm. As it is shown in Table 3 and Table 4, the Bayesian Regularization algorithm has the lowest MSE for propane and butane. Therefore, it was the one selected in this study. The MSE values for these two substances were $2.29 \cdot 10^{-4}$ and $4.63 \cdot 10^{-5}$, respectively.

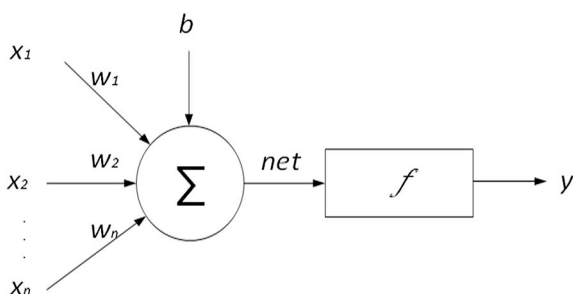


Fig. 2. Feedforward neural network.

3.2. Optimizing neurons number

The determination of the neurons' number is essential. Considering few neurons causes underfitting and, contrarily, overfitting can occur if the number of neurons is higher than a specific value. In this study, an ANN was trained based on Bayesian Regularization BP algorithm for propane and butane. The number of neurons was varied from 1 to 20, and an optimum number of neurons was chosen based on the minimum value of MSE of the training. According to Fig. 3, the optimum number of neurons for propane and butane were five and four, respectively. The minimum values of MSE for propane and butane were 0.00025 and 0.000129, respectively, which were lower than 0.001, taken as a sufficient threshold value for the mean square error.

3.3. ANN setup and results

For solving the problem, a multilayer feed forward neural network was used. A general picture of this method has been depicted in Fig. 4. The multilayer feed forward network consists of three layers. The first one is the input layer through which the data (i.e., filling level and temperature just before the explosion as input parameters) are imported into the network, and the last layer is the output one, i.e., mechanical energy per cubic meter of the vessel as output data, which gives the target data (with this mechanical energy per cubic meter and the vessel volume, the mechanical energy released by the explosion can be calculated). Between these two mentioned layers, there is another hidden one. The number of hidden layers depends on the accuracy that is required for a particular problem. In this analysis, the number of hidden layers was set to one, which provided reasonable accuracy. Based on the neurons optimization process, the number of neurons at the hidden layer was five in the case of propane and four in the case of butane. The transfer function applied in this layer was a sigmoid, because it had an easy and straightforward differentiation for using in the back-propagation algorithm. For the output layer, the number of neurons had to be one in both cases, and the transfer function was *purelin* (linear).

The process was performed with the MATLAB Neural Network toolbox version R20015a (8.5.0.197613 – License Number: 107001). The number of input data for the training process was 121 and 201 for propane and butane, respectively. It reached a convergence level after 348 iterations in the case of propane and 191 iterations with butane. The validation process was done with 15% of the data to check the network generalization. The resulting network was tested with 15% of the data to provide an independent measure of the network performance during and after training. In the training process, a part of the available data was used to train the network and find out the suitable weights and biases. These quantities were checked in the validation process. Based on the obtained results, it would be preferred to choose 15% of data randomly, which finally gave good results. The final results also demonstrated a good level of performance according to the prepared dataset (Beale et al., 2010).

For propane, the designed network regression R values were close to one, showing that there was a close correlation between ANN outputs and target values from prepared dataset. Fig. 5 shows how much accurate the ANN model is.

Also, the optimized weights for propane produced by the artificial neural network model are summarized in Table 5.

In the case of butane, the regression results (Fig. 6) show that the network was appropriately trained and a linear relation exists between output and target data. R values were close to unity which indicated linearity between target values from prepared dataset and ANN output data.

The optimal weights for butane from the artificial neural network between input and hidden layers ($W1$) and between hidden and output layers ($W2$) are shown in Table 6.

Table 3

Backpropagation training algorithms for propane.

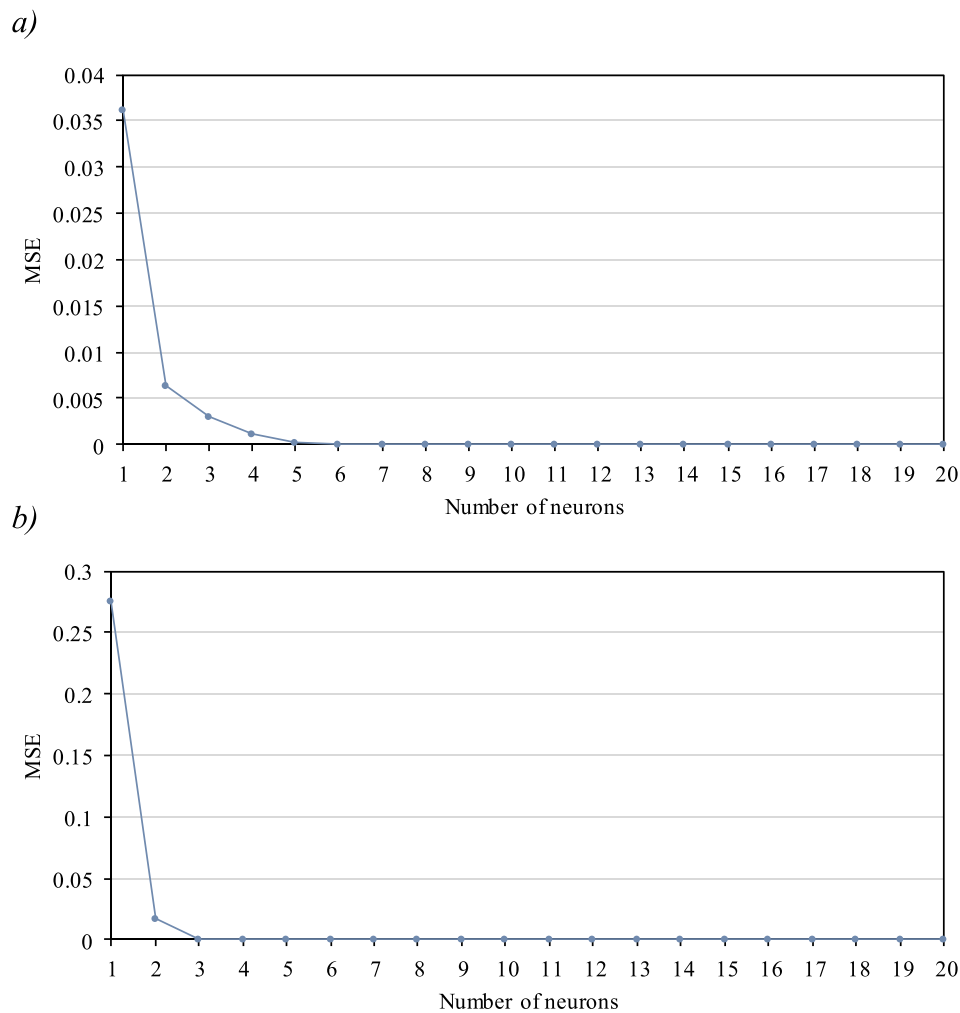
Backpropagation algorithm	Function	Testing mean square error (MSE)	Epoch ^a	Regression R value	Best linear equation
Levenberg-Marquardt backpropagation	<i>trainlm</i>	0.000364	232	0.99996	$Output = 1 \cdot Target + 0.0049$
Bayesian Regularization	<i>trainbr</i>	0.000229	385	0.99998	$Output = 1 \cdot Target + 0.00098$
Scaled Conjugate Gradient	<i>trainscg</i>	0.0736	39	0.99205	$Output = 0.97 \cdot Target + 0.17$

^a In training process, each level is called “training epoch”. All the inputs are entered in each training epoch and give outputs which are compared with the target to give the error. By this process, weights and biases are calculated and modified at each epoch.

Table 4

Backpropagation training algorithms for butane.

Backpropagation algorithm	Function	Testing mean square error (MSE)	Epoch	Regression R value	Best linear equation
Levenberg-Marquardt backpropagation	<i>trainlm</i>	$5.85 \cdot 10^{-5}$	116	1	$Output = 1 \cdot Target + 0.0019$
Bayesian Regularization	<i>trainbr</i>	$4.63 \cdot 10^{-5}$	1000	0.99999	$Output = 1 \cdot Target - 0.0012$
Scaled Conjugate Gradient	<i>trainscg</i>	$8.39 \cdot 10^{-1}$	17	0.94398	$Output = 0.93 \cdot Target + 0.33$

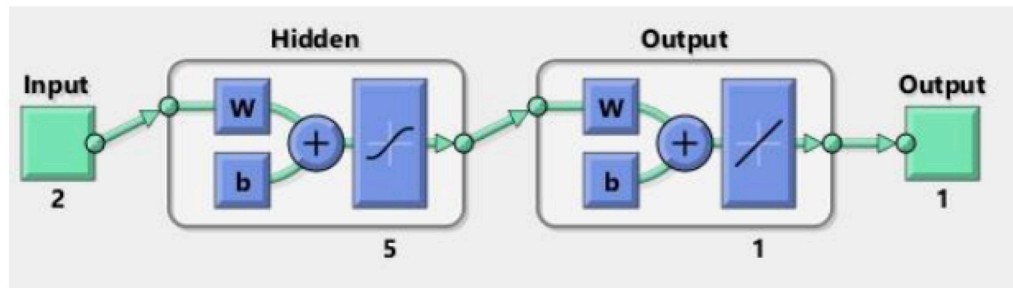
**Fig. 3.** Optimized neurons number for: a) propane, b) butane.

3.4. Comparative study

Root-Mean-Square Deviation (RMSD) (Piñeiro et al., 2008) as a statistical toolkit was used in the comparison of the results obtained with the ANN method and the aforementioned experimental data from Birk and VanderSteen (2006); Birk et al. (2007) and Johnson et al. (1990). TNT equivalent mass and the well-known plot of the scaled distance vs.

peak overpressure were utilized for obtaining the resulting overpressures (ΔP) at different distances. The results are shown in Table 7, together with those obtained from polynomial expressions (Hemmatian et al., 2017b). As can be seen, the functions derived from the ANN show a good performance. It can be stated that both methods proposed are accurate and practical to be applied. The nonlinear relation between temperature and filling level (Hemmatian et al., 2017b) is probably the

a)



b)

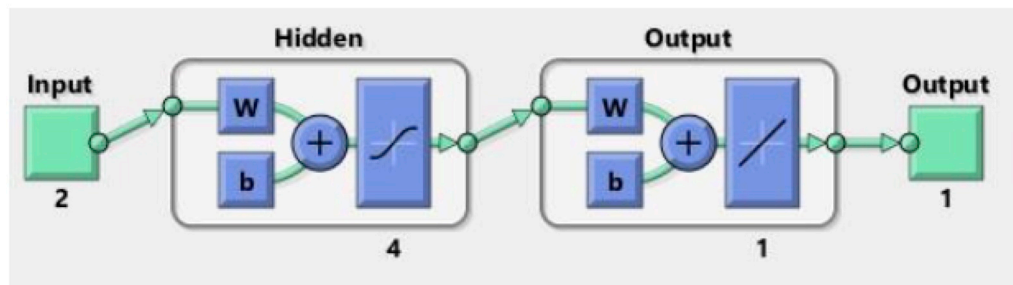


Fig. 4. Artificial neural network structure for: a) propane, b) butane.

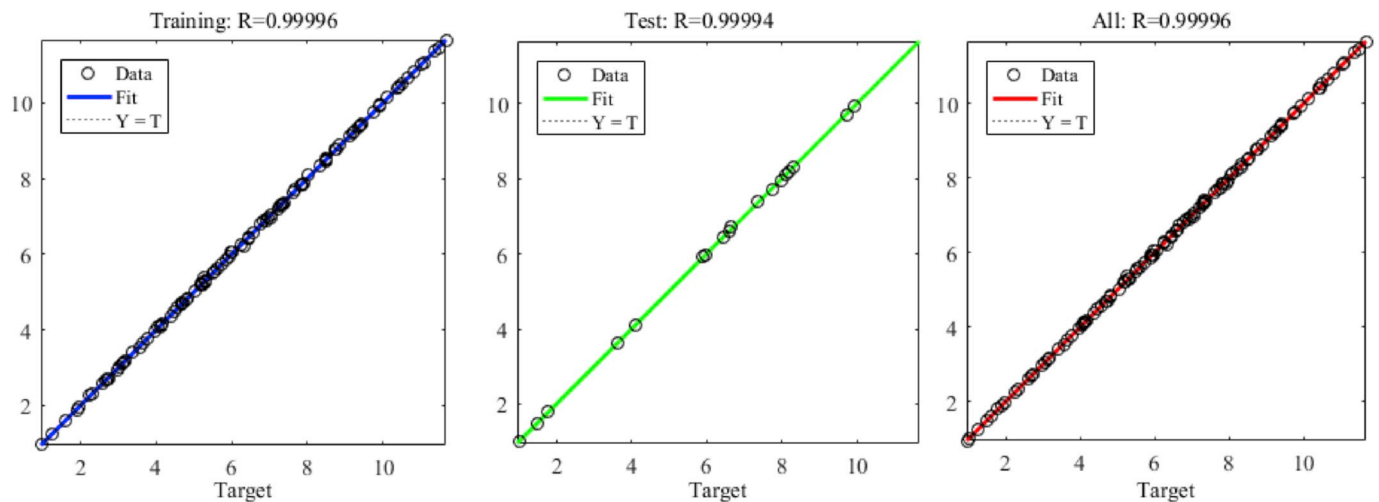


Fig. 5. Regression plots of the mechanical energy (MJ) per cubic meter of the vessel for propane. Left: during training; middle: during the testing; right: all the data including validation. (Abscissa: target values from prepared dataset – Ordinate: ANN outputs).

Table 5
Propane's weights matrix.

Neuron	W1		W2
	Input variables		Output
	Temperature	Filling level	Energy
1	−1.2335	−0.2862	−0.8641
2	1.7512	0.3928	0.5474
3	−0.8560	0.2377	3.16
4	1.2560	−0.3420	1.1380
5	1.1617	0.2995	1.1103

W1: Weights between input and hidden layers.

W2: Weights between hidden and output layers.

reason for the observed deviation that, as seen in the comparative analysis, remains in the range of the expected accuracy of this type of calculation and, therefore, should be considered acceptable. Fig. 7 shows the differences between the various approaches and the experimental values. At short distances (corresponding to high overpressures) the calculated values from the four approaches are higher than the experimental ones. This should be attributed to the use of the TNT equivalency method for the estimation of the peak overpressure: this method gives usually better results in the far field, while it often overpredicts them in the near field.

3.4.1. Example of application

A cylindrical vessel with a volume of 80 m³, initially filled to 58% with liquid propane at room temperature (20 °C and 8.4 bar), undergoes

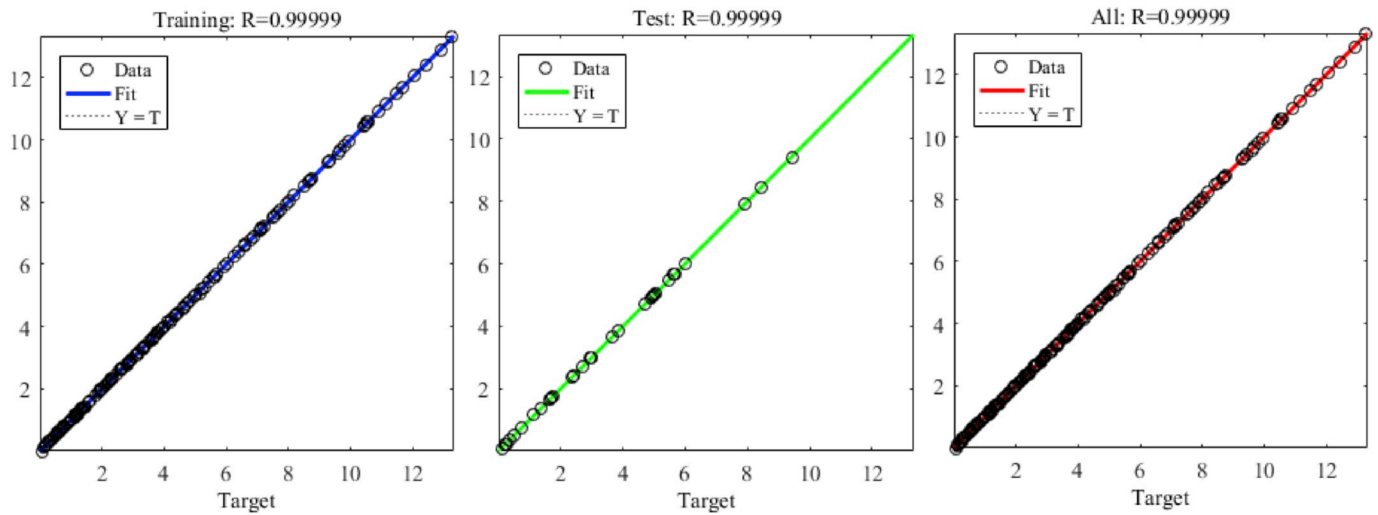


Fig. 6. Regression plots of the mechanical energy (MJ) per cubic meter of the vessel for butane. Left: during training; middle: during the testing; right: all the data including validation. (Abscissa: target values from prepared dataset – Ordinate: ANN outputs).

Table 6

Butane's weights matrix.

Neuron	W1		W2
	Input variables		Output
	Temperature	Filling level	Energy
1	-1.3757	-0.4138	-0.2668
2	0.7913	-0.1637	-1.8164
3	-0.8212	-0.1932	-2.4487
4	-1.5521	0.4522	-0.3672

W1: Weights between input and hidden layers.

W2: Weights between hidden and output layers.

Table 7

RMSD values for the comparison of ΔP experimental values and the prediction from the different methodologies and the TNT equivalency method.

Thermodynamic assumption ^a				
RMSD	RAIE	SE	Polynomial approach	Neural Net Fitting approach
Johnson-TNT eq. method	2.3	2.2	2.2	2.2
Birk-TNT eq. method	4.9	4.1	4.2	4.3

^a RAIE = Real gas behavior and adiabatic irreversible expansion; SE = Liquid superheating energy.

a BLEVE due to fire engulfment, when the content temperature is 50 °C. The filling degree is 34% at the burst moment. Estimate overpressure (ΔP) at a distance of 100 m (Hemmatian et al., 2017b).

The MATLAB file for calculating the overpressure in kPa is:

```
clear
clc
T = input('Temperature(K)\n'); %Temperature just before the
explosionfl = input('Filling Level\n'); %Filling level just before
the explosion
d = input('Distance(m)\n');
v = input('Volume(m3)\n'); %Volume of vessel
a = [T; fl];
Energy_predicted_per_m3 = propanepredictor3(a);
Energy_predicted = Energy_predicted_per_m3*v; w_tnt=((10^3)
*0.4)/4680)*Energy_predicted;
c = w_tnt^(1./3);
scaled_distance = d/c;
```

(continued on next column)

(continued)

```
overpressure_kPa=((1/scaled_distance)+(4/
(scaled_distance^2))+(12/(scaled_distance^3)))*101.32;
name = 'Overpressure';
X = [name, ' is equal to ', num2str(overpressure_kPa), ' kPa']; disp
(X)
```

Here is the procedure for calculating the example and the result in kPa when running the previous MATLAB file:

```
Temperature (K)
323.15
Filling Level
0.34
Distance (m)
100
Volume (m3)
80
Overpressure is equal to 3.6435 kPa.
```

4. Conclusion

The artificial neural network (ANN) approach was used to find the appropriate function between temperature and filling level as input data and the mechanical energy invested in creating the BLEVE peak overpressure as output data. Calculations were performed by assuming real gas behavior and adiabatic irreversible expansion, as this thermodynamic assumption provides more accurate and therefore realistic predictions than the others.

Two functions were generated for propane and butane by using ANN. The smallest minimum square error (MSE) was given by three-layer Bayesian Regularization backpropagation algorithm with tangent sigmoid transfer function (*tansig*) at the hidden layer and linear transfer function (*purelin*) at output layer. For both substances, the designed networks regression R values were close to 1, this meaning that there was a close correlation between outputs and targets.

To check the results from the ANN networks with two sets of experimental data from the literature, the corresponding peak overpressure values were obtained by applying the TNT equivalency method. According to the root mean square deviation (RMSD), calculated by various methodologies, the ANN networks showed a good level of performance (although there was a discrepancy in the near field for all the four applied methodologies). This, combined with its simplicity, allows obtaining quick and accurate results in an easy way. This

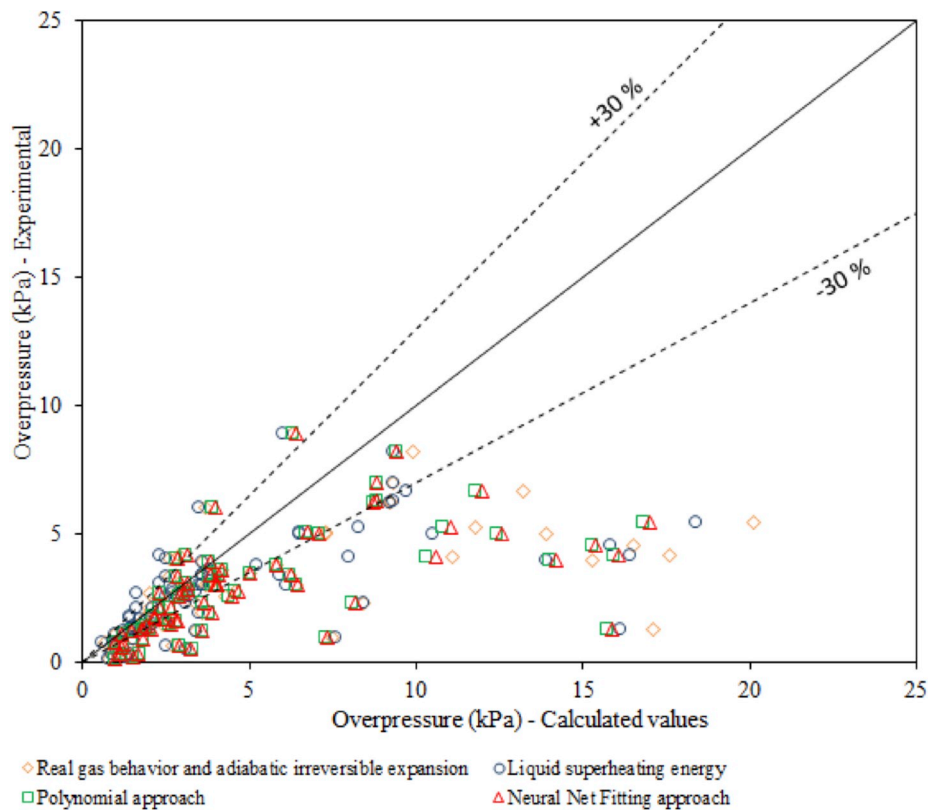


Fig. 7. Results from the different methodologies vs the ΔP experimental values.

methodology for calculating the mechanical energy is independent of substance's thermodynamic properties information (enthalpy, entropy, internal energy, etc), and it only requires the vessel filling level and temperature just before the explosion, and the vessel volume, as input parameters to calculate the BLEVE mechanical energy.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jlp.2019.104021>.

Nomenclature

b	Bias value
\mathbf{b}	Bias vector
f	Transfer function
m	Mass (kg)
P_{rup}	Failure pressure (kPa)
T	Temperature (K)
V	Volume (m^3)
w	Weight value
W	Weight matrix
x_i	Input variable
y	Output variable
Y	Output vector

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