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## A Completed State Equations Model for the Simulation of Compression and Expansion of Gases- Application to Air and Hydrogen.

**Alfred Rufer**

### **Abstract**

For modeling the compression and expansion of gases many different state equations can be used when the mechanical variables of compressors and expansion machines are simulated. The present paper simulates and compares different methods based on state equations combined with an integrated thermal model. The simplest model uses simple expressions where only the volumetric ratio is considered. Then different ways to use more complex state equations are presented for the simulation of non-ideal gases like hydrogen. The Van der Waals and the Beattie Bridgeman state equations take in account the attraction forces between molecules and the volume occupied by them. The simulations represent the phenomena in a specific piston cylinder system. Air and hydrogen compressions are defined between 15 and 160 bar. The behaviour in expansion mode is simulated with the same assembly, but where an intake action at constant pressure is realized during a first section of the stroke and which is followed by a real expansion process during the remaining part of the same stroke by closing the intake valve.

**Keywords:** Gas compression, Gas expansion, State equations, Simulation model, Hydrogen.

### **1. Introduction**

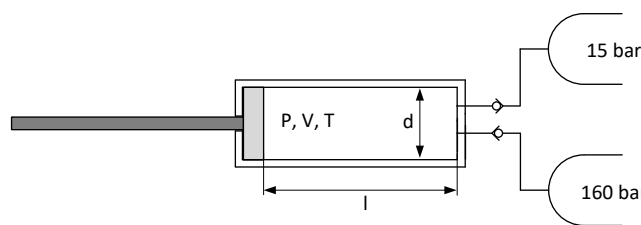
Against the backdrop of issues related to environmental problems and climate change, many alternative solutions to classical equipment and renewable energies are proposed with the goal to limit or reduce the greenhouse gas emissions. When several of the new energy sources present their characteristic of intermittency or stochastic availability, energy storage technologies have to be strongly developed and integrated into the new systems. Nowadays battery energy storage systems are at the front of interests with their still increasing energy density and their high-power capability. But regarding the lifecycle of electrochemical solutions or their capability to store energy amounts compatible with the needed quantities for a seasonal storage, several questions are still open, from the technical and from the economic point of view. Consequently, alternative solutions are proposed with the example of compressed air energy storage (CAES) where the technology can be designed for a high number of cycles up to 10'000 to 15'000 cycles or where the equipment can be repaired after ageing problems occur. Another technique which would help to store huge quantities of energy for a shift of solar PV power from summer to winter is based on a transformation into a chemical carrier like hydrogen or other synthetic fuels. Concerning Hydrogen, but this is also valid for different gases, a significant density of energy can only be achieved through a compression process. And the energetic performance of gas compression and expansion systems has never been at the front of industrial developments up today. High pressure compression stations often use a cascade of compressors like air-driven gas boosters, leading to aberrant results [1]. Tentative solutions for an increased efficiency have been proposed [2-7], where as well the actuator principle as the compression cylinders themselves have been modified. In addition to the studied compression machines, an expansion system to be used as an expansion work recovery system for fuel-cell trucks has also been analysed [8]. In nearly all new proposals, the compression and expansion process have been described on the base of relations valid for ideal gases. This assumption can be used for a gas like air, but

the question of the validity of the models for other real gases like Hydrogen is open. In the present paper, the behaviour of a piston- cylinder assembly is analysed in compression and expansion modes with different equations of state as the Van der Waals model or other multiple parameter polynomial models for the evaluation of the resultant pressure and temperature. Sophisticated models as available in powerful computer programs give accurate results regarding the thermodynamic states of different gases [9] but the simple formalisms like the classical Van der Waals equations can be simply integrated in simulations where the mechanical variables of compression and expansion cylinders and coupled driving mechanisms are of major interest. Adiabatic and isothermal compression processes are simulated and compared. Further on, a thermal model is used complementarily to and in the loop of the state equations for an evaluation of the gas temperature.

**2 Structure and dimensions for the simulation of the compression/expansion cylinder**

**2.1 Compression**

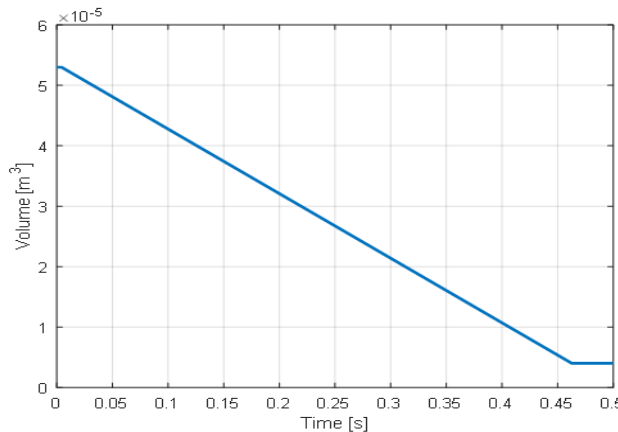
For the different simulations with the different models a specific piston-cylinder is used. The comparison study is based on an implementation of the physical elements and of the different thermodynamic state equations in a dynamic time-based representation where the velocity of the piston is imposed (Simulink). The dimensions and other parameters have been used in a previous study [5]. The simple piston-cylinder assembly is represented in Fig. 1 together with the inlet pressure reservoir at 15 bar and the output receiver at 160 bar. Anti-return valves are placed between the reservoirs and the compression cylinder. P, V, and T are the variables and d (inner diameter, 27.5 mm in the example) and l (stroke, 90 mm in the example) are the parameters of the cylinder. The volume of the cylinder is varied from the maximum value  $V_{cyl}$  at BDC (Bottom Dead Center) down to the lowest value at the TDC (Top Dead Center) with a velocity of  $vel = 0.18$  m/s. The evolution of the volume in function of time is represented in Fig. 2. A lower limit of the volume is introduced in order to avoid problems in the calculation of the volume ratio (no division by 0).



**Fig. 1:** Compression piston-cylinder system.

$$V_{cyl} = \pi \cdot d^2 / 4 \cdot l = \pi \cdot (27.5)^2 / 4 \cdot 90 = 53456 \text{ mm}^3 \text{ or } 53.5 \cdot 10^{-6} \text{ m}^3 \tag{1}$$

$$vel = l / 0.5 \text{ s} = 0.090 \text{ m} / 0.5 \text{ s} = 0.18 \text{ m} / \text{s} \tag{2}$$



**Fig. 2:** Evolution of the volume of the compression cylinder.

**2.1.1. Compression curves of air and hydrogen**

A classical expression for the evolution of the pressure of an ideal gas in dependency of the variation of the volume is given in eq. (3). This expression has been used for the compression of air in adiabatic ( $\gamma = 1.4$ ) and in isothermal

conditions ( $\gamma = 1$ ). The two curves are represented in Fig. 3. According to the experimental set-up shown in Fig. 1 the pressure in the cylinder varies from the intake level of 15 bar to the pressure in the output reservoir of 160 bar.

$$P_{gas} = P_{in\_gas} \left( \frac{V_{comp\_max}}{V_{compr\_var}} \right)^\gamma \tag{3}$$

with  $\gamma = 1.4$  in adiabatic mode and  $\gamma = 1$  in isothermal.

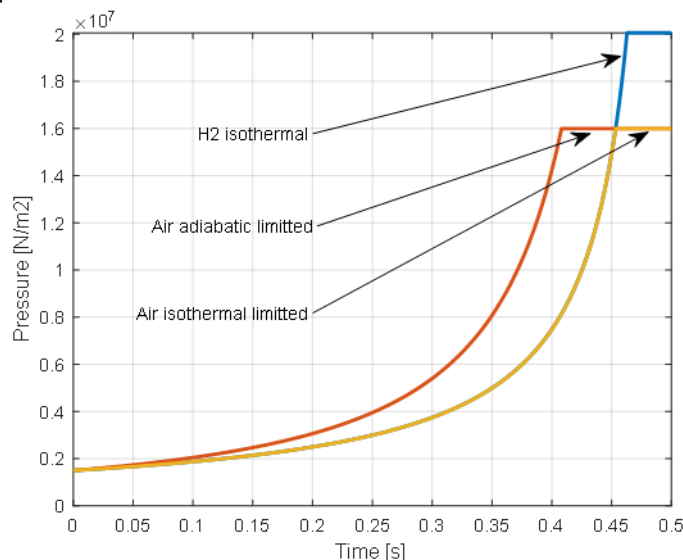


Fig. 3: Comparison of compression curves.

For a non-ideal gas like Hydrogen, different equations of state can be used. A first relation directly deduced from the ideal gas law is used (eq. 4) and the corresponding curve is compared with the curve of the isothermal compression of eq. (3). The ideal gas law is a representation of the compression phenomenon supposing an inverse proportionality between pressure and volume.

$$P = \frac{R \cdot T}{v} = \frac{m \cdot R \cdot T}{V} \tag{4}$$

In this expression for the pressure  $P$  the mass volume  $v$  or the real volume  $V$  can be used. The functional diagram of Fig. 4 is implemented for the representation of the evolution of the pressure.

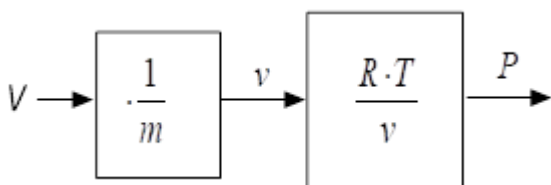


Fig. 4: Functional diagram of the ideal gas law model

In opposition to the eq. (3) where only the initial pressure and the geometric (volumetric) conditions are considered, the ideal gas law uses the mass  $m$  of gas and the related gas constant  $R$ . The temperature is supposed to be known. The mass of Hydrogen sucked from the primary reservoir (15 bar) is calculated with the same relation (4) and the parameters of the cylinder represented in Fig. 1:

$$m = \frac{P \cdot V}{R \cdot T} = \frac{15 \cdot 10^5 \text{ N/m}^2 \cdot 53.5 \cdot 10^{-6} \text{ m}^3}{4.124 \text{ kJ/(kg} \cdot \text{K)} \cdot 293 \text{ K}} = 0.664 \cdot 10^{-4} \text{ kg} \tag{5}$$

The Hydrogen related constant  $R$  being:

$$R = 4.124 \text{ kJ/(kg} \cdot \text{K)} \tag{6}$$

A compression curve of Hydrogen is calculated according to eq. (4) under isothermal conditions and is represented in Fig. 3. This curve (blue curve) is identical to the curve of the isothermal compression of air calculated with eq. (3) (yellow curve). The upper limit of the yellow curve is imposed as an upper pressure limit (160 bar). The blue curve represented reaches a different-upper limit. This value is related to the lowest value of the volume as represented in Fig. 2.

**2.2. Two other state equations for non-ideal gases**

Two other equations of state are considered which are supposed to bring a more accurate representation of the evolution of the pressure. First the Van der Waals state equation is considered. and further a still more complex model is given by the Beattie-Bridgeman state equation [10].

**2.2.1. State equation of Van der Waals**

The Van der Waals state equation is an improvement of the ideal gas equation where the attraction force between molecules is introduced (term  $a/v^2$ ). The volume occupied by the molecules (term  $b$ ) is also considered. The expression for the pressure gives:

$$P = \frac{R \cdot T}{v - b} - \frac{a}{v^2} \tag{7}$$

The mass volume  $v$  is calculated from the system variable  $V$  (the real volume).

$$v = \frac{V}{m} \tag{8}$$

and the factors  $a$  and  $b$  are given through:

$$a = \frac{27R^2 \cdot T_{cr}^2}{64P_{cr}} \quad \text{and} \quad b = \frac{R \cdot T_{cr}}{8P_{cr}} \tag{9}$$

$a$  and  $b$  are calculated with the parameters of Table 1 [10].

Table 1: Constants of Hydrogen for the Van der Waals model.

	Formula	Molar mass M Kg/kmol	Constant R kJ/kg*K	T <sub>cr</sub> K	P <sub>cr</sub> MPa	Vol m <sup>3</sup> /kmol
Hydrogen (normal)	H <sub>2</sub>	2.016	4.124	33.3	1.3	0.0649

The corresponding functional diagram of the Van de Waals model is represented in Fig. 5

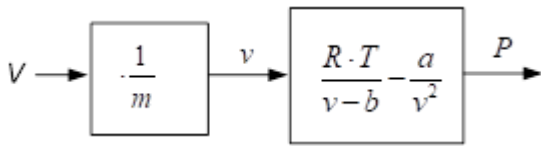


Fig. 5: Functional diagram of the Van der Waals model.

**2.2.2. State equation of Beattie-Bridgeman**

The state equation of Beattie-Bridgeman is based on five constants which are determined experimentally. The expression of the pressure is given by eq. (10)

$$P = \frac{R_u \cdot T}{\bar{v}^2} \left( 1 - \frac{c}{\bar{v} \cdot T^3} \right) (\bar{v} + B) - \frac{A}{\bar{v}^2} \tag{10}$$

Table 2: Constants for the Beattie-Bridgeman state equation.

	A <sub>0</sub>	a	B <sub>0</sub>	b	c
Hydrogen H <sub>2</sub>	20.017	-0.00506	0.02096	-0.04359	504

Finally, the implementation in the simulation is done according to the functional diagram of Fig. 6.

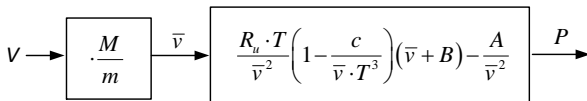


Fig. 6: Functional diagram of the Beattie-Bridgeman model.

In Fig. 7 three compression curves for Hydrogen are represented namely an ideal gas law curve (red curve), a Van der Waals model curve (yellow curve) and a Beattie-Bridgeman model curve (blue curve). In this simulation, the pressure limits are given through the lower volume limit (See Fig. 2). For pressure values under 50 bar, the difference between models is limited. Only for higher values of the pressure (above 50 to 100 bar) the difference becomes significant.

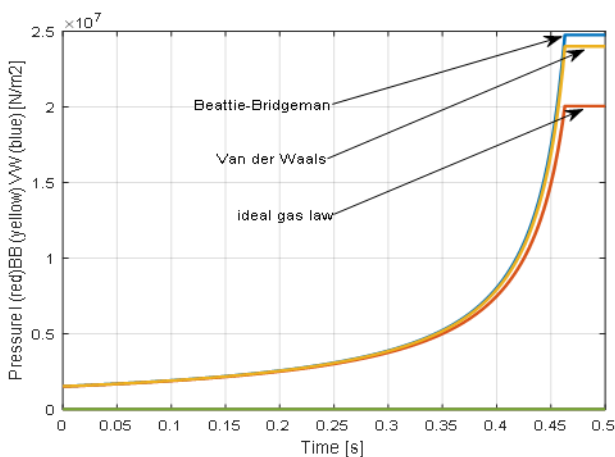


Fig. 7: Different compression curves

**2.2.2. Calculation of the temperature**

$$A = A_0 \left( 1 - \frac{a}{\bar{v}} \right) \quad \text{and} \quad B = B_0 \left( 1 - \frac{b}{\bar{v}} \right) \tag{11}$$

where

The input variable of eq. (10) is the molar volume  $\bar{v}$  and it is calculated from the mass volume  $v$  according to

$$\bar{v} = M \cdot v = M \cdot V / m \tag{12}$$

where  $M$  is the molar mass

The universal gas constant  $R_u$  is recalculated from the specific gas constant  $R$

$$R_u = M \cdot R \tag{13}$$

The parameters for Hydrogen are given in Table 2 [10].

For the calculation of the evolution of the temperature during compression the relation (3) is completed by another analytic equation which considers the variation of the volume (eq. (14):

$$T_{gas} = \frac{T_{in}}{\left( \frac{V_{compr\_var}}{V_{comp\_max}} \right)^{\gamma-1}} \tag{14}$$

So the pressure and the temperature of the gas can be calculated with the global model as represented in Fig. 8, where the two analytic expressions are used together. In this model, the thermal conditions of the evolution are represented through the polytropic exponent  $\gamma$ .

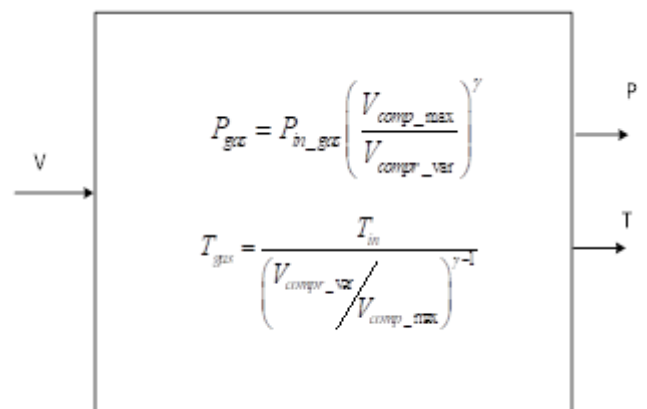
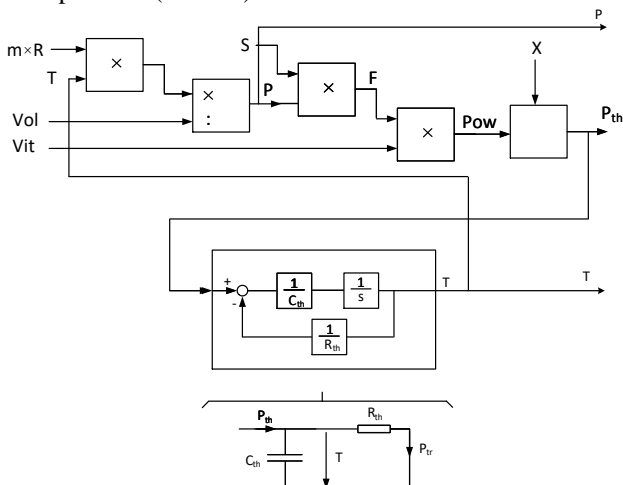


Fig. 8: The analytic model for pressure and temperature

Another method we call “The Thermal Integrated Model (TIM)” will be particularly useful in relation with the use of the two complex state equation (Van de Waals and Beattie-Bridgeman). This method includes a thermal model based on a thermal equivalent circuit where the thermal capacity of

the mass of the gas  $C_{th}$  and a thermal resistor  $R_{th}$  are used.  $R_{th}$  represents the heat flow from the compressed gas towards the surrounding. The thermal model is used “in the loop” together with the state equation of the gas. This new TIM representation allows to calculate the simultaneous and coupled evolution of the pressure and of the temperature during compression.

The evaluation of the temperature using the thermal equivalent circuit supposes that the input variable of this circuit (the thermal power) is known. This variable is calculated as the mechanical power transmitted to the cylinder by the external force  $F$  as long as no gas is transferred from the cylinder to the reservoir. The force is calculated as the product of the pressure multiplied by the piston’s surface  $S$ . Further the product of the force by the imposed velocity of the piston gives the mechanical power  $Pow$ . (Fig. 9). In Fig. 9 a binary variable  $X$  intervenes in the functional block between the mechanical power  $Pow$  and the thermal power  $P_{th}$ . This variable sets the condition that all the mechanical power is transmitted to the mass of gas as long as the exhaust valve remains closed. As soon as this valve opens the mechanical power no more contributes to the elevation of the temperature of the gas, but “moves” the compressed gas to the exhaust reservoir at a constant value of the pressure (160 bar).



**Fig. 9:** TIM Model with the thermal functional diagram “in the loop”

2.2.3. Comparison of results

First, the evolution of the pressure during compression which is calculated with the analytic model is compared to the evolution calculated with the TIM model. The compressed gas is in this first case air. The TIM model uses the ideal gas law (Fig. 9). The adiabatic compression is modelled with an exponent  $\gamma = 1.4$  in the analytic model and with an infinite value of the thermal resistance  $R_{th}$  in the TIM model. The feedback  $1/R_{th}$  in the diagram is disconnected in this case.

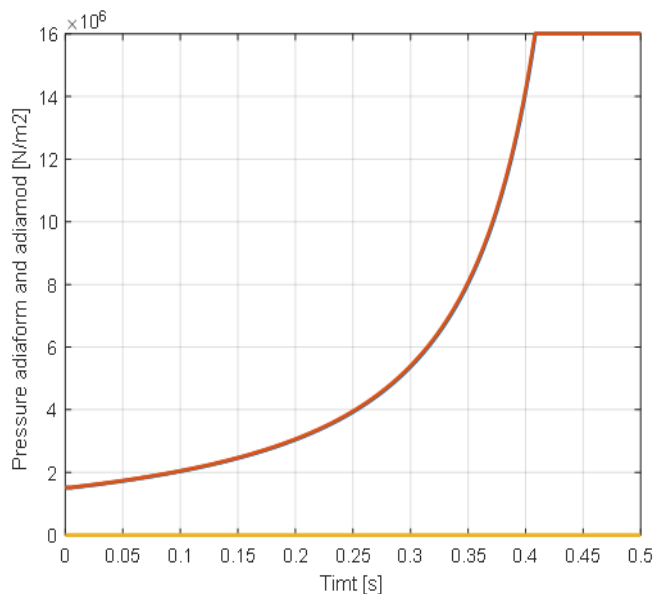
For the thermal capacity  $C_{th}$  eq. (16) is used with a mass of air equal to:

$$m = \frac{p \cdot V}{R \cdot T} = \frac{15 \cdot 10^5 \text{ N/m}^2 \cdot 53.5 \cdot 10^{-6} \text{ m}^3}{0.287 \text{ kJ/(kg} \cdot \text{K)} \cdot 293 \text{ K}} = 9.54 \cdot 10^{-4} \text{ kg} \tag{15}$$

$$C_{th} = m \cdot c_v = 9.54 \cdot 10^{-4} \text{ kg} \cdot 0.718 \text{ kJ/(kg} \cdot \text{K)} = 0.682 \text{ J/K} \tag{16}$$

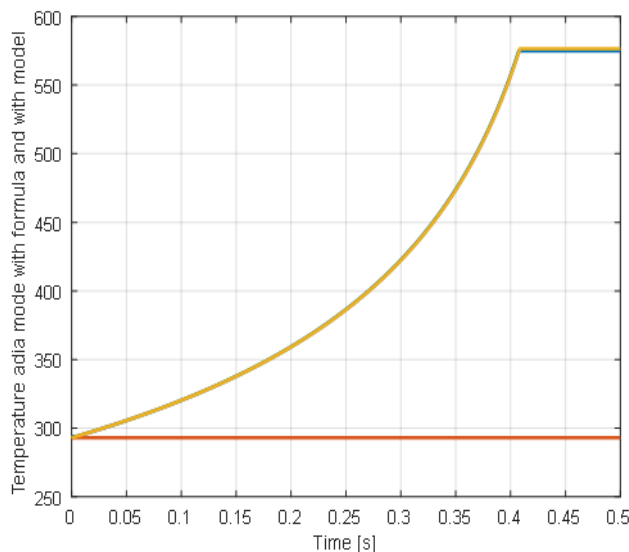
The two pressure curves are represented in Fig. 10. The

curves are nearly superposed (blue curve and red curve) showing the equivalence of the two models.



**Fig. 10:** Pressures in adiabatic mode with the analytic formula (eq. 3) and with the TIM model (air, Fig. 9). (The blue and red curves are practically superposed).

A comparison of the curves for the temperature is also done (eq. 14 and Fig. 9) and is represented in Fig. 11. The values are here also similar (575.0 K for the analytic model and 576.6 for the TIM model).



**Fig. 11:** Temperatures in adiabatic mode with the analytic formula (blue curve) and with the TIM model (air) (yellow curve). The red curve represents the isothermal case.

A further comparison of models is made for the compression of Hydrogen. In this case, two TIM models are compared namely a TIM model using the Van der Waals state equation and a TIM model using the Beattie-Bridgeman state equations. The TIM model with Van der Waals state equation is represented in Fig. 12 and the TIM model with Beattie-Bridgeman state equation is represented in Fig. 13. In these diagrams, the pressure during compression is calculated from the volume (or mass volume) with the help of the state equation. In these equations, the temperature is involved and needs an additional evaluation for it. From the

pressure, the compression force is evidently calculated, and then, the compression mechanical power is calculated by multiplication of the force by the piston's velocity. As long as the exhaust valve is closed, the mechanical power is transmitted to the gas in form of heat. The mechanical power can be used as input variable of the thermal model based on

$$C_{th_{H_2}} = m \cdot c_v = 0.664 \cdot 10^{-4} \text{ kg} \cdot 10.16 \text{ J}/(\text{g} \cdot \text{K}) = 0.664 \cdot 10^{-1} \text{ g} \cdot 10.16 \text{ J}/(\text{g} \cdot \text{K}) = 0.674 \text{ J/K} \tag{17}$$

The thermal capacity of the Hydrogen mass (in the initial volume and at initial pressure) is similar to the thermal capacity of air (identic volume and pressure). This is due to a much higher mass of air (0.954g) than hydrogen (0.06g) when the massic heat values are in inverse proportions (0.718J/gK for air versus 10.1J/gK for H<sub>2</sub>).

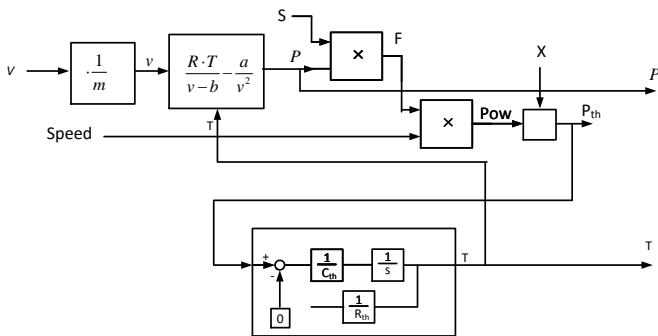


Fig. 12: TIM model with Van der Waals state equation.

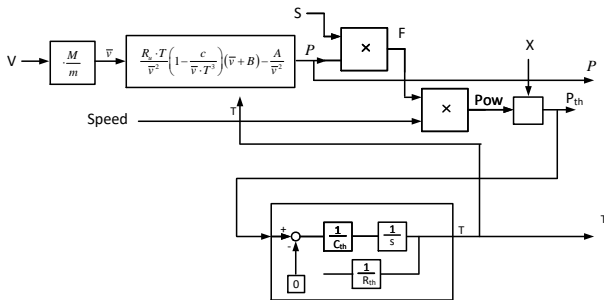


Fig. 13: TIM model with Beattie-Bridgeman state equation

The pressure curves of the two TIM models are represented in Figure 14 and are totally superposed. When these curves are compared with the evolution of the pressure calculated with the analytic model (Fig. 10), one can see that the pressure value of 160bar is reached in these cases earlier (0,4s instead of 0.41s).

thermal capacity and thermal resistance for the heat flow to the surrounding. In the thermal model, the disconnection of the feedback (1/Rth) and replacing it by the value of zero corresponds to an adiabatic characteristic. The thermal capacity is in this case (Hydrogen):

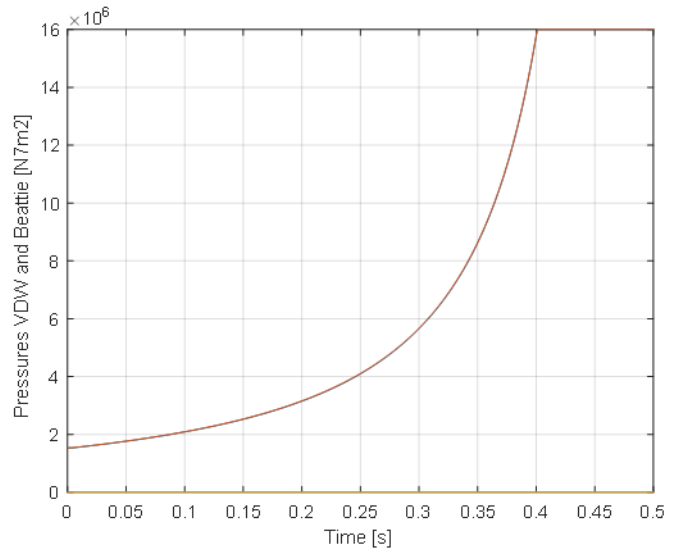


Fig. 14: Pressures H<sub>2</sub> adiabatic VDW and Beattie (totally superposed curves)

Regarding the evolution of the temperature, the same remarks are valid as for the pressure (same values, and earlier reach of the limit). The temperature curves calculated with the Van de Waals model and with the Beattie-Bridgeman models are represented in Fig. 15.

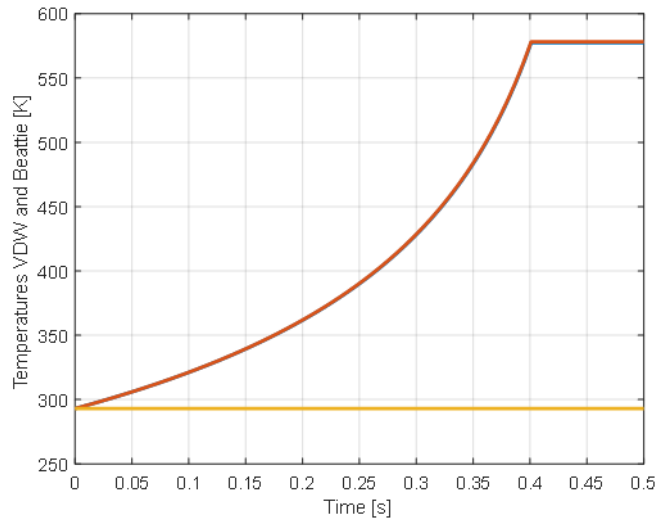
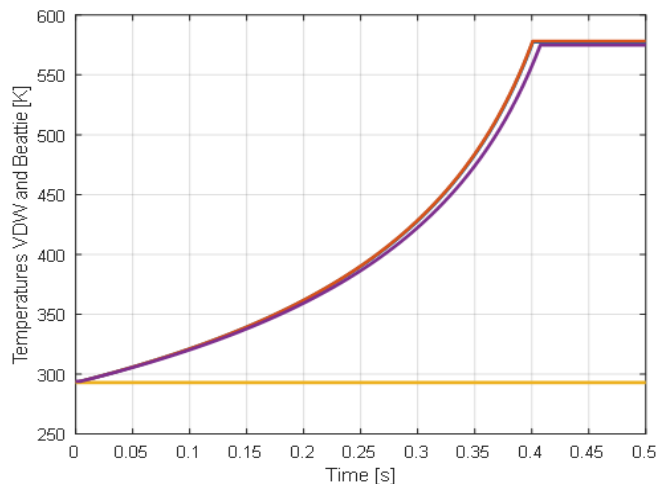


Fig. 15: Curves for the temperature of Hydrogen, Van der Waals (blue curve) and Beattie-Bridgeman (red curve) TIM models. The yellow curve corresponds to the isothermal case.

The delay of reaching the pressure limit between the analytic model and the two TIM models (VDW and B-B state equations) can be seen on the curves in Fig. 16.

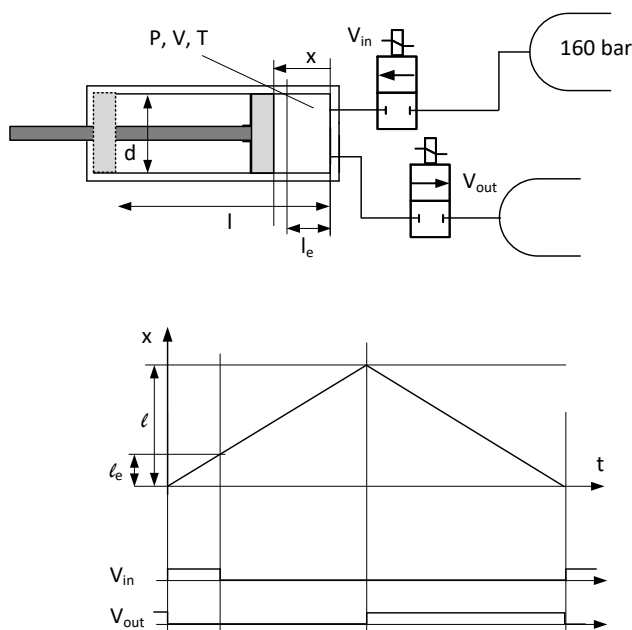


**Fig. 16:** Temperatures H<sub>2</sub> adia VDW and Beattie (red, superposed) and comparison with the analytic model (blue curve). The yellow curve corresponds to the isothermal case.

**2.3. Expansion**

For the simulation of the expansion phenomenon the same cylinder as for compression is used. The system used for the expansion is represented in Fig. 17. The intake of the high-pressure gas is controlled with the intake valve  $V_{in}$  and the exhaust by the valve  $V_{out}$ . The control of the valves is represented in the lower diagram of Fig. 17. The expansion from an initial pressure of 160 bar is simulated. The volumetric expansion is defined with a ratio of 1 to 3. For that the gas is injected in the cylinder during the first third of the stroke from a reservoir with constant pressure. The position  $x$  of the piston evolves from zero up to the position

le. Then, the inlet valve is closed during the remaining two thirds of the same stroke. The position of the piston is increased up to the full length of the stroke. As a result, the volume of the gas increases. During these three thirds of the positive stroke the exhaust valve is closed. Then during the return stroke the expanded gas is exported through the opened exhaust valve  $V_{out}$  to the exhaust reservoir. In order to prevent when the opening of the exhaust valve from an additional dynamic transient the pressure of the exhaust reservoir is supposed to correspond to the pressure level after expansion.



**Fig. 17:** Structure of the expansion cylinder with sequential diagram of the control of the valves.

**2.3.1 Numeric values for the simulation of the expansion phenomenon**

The maximum volume of the cylinder is identical to the previous value according to rel. (1), namely

$$V_{cyl} = 53.5 \cdot 10^{-6} m^3$$

The volume of the intaken gas at high pressure (first third of the stroke) becomes

$$V_e = 53.5 \cdot 10^{-6} m^3 / 3 = 17.83 \cdot 10^{-6} m^3$$

The expansion velocity has in this case the same value as for the compression but with an opposite sign, namely -0.18m/s. The duration of the intake is 0.5s/3 or 0.166s. The evolution of the gas volume inside of the cylinder is represented in Fig. 18. Between 0 and 0.166 s, the constant value of the volume does not illustrate the real volume of the cylinder, but means that the cylinder is filled with gas under constant pressure up to the indicated value of the volume. The resultant expansion ratio is represented in Fig. 19 where the value of 1 is

characteristic of the filling duration (0 - 0.166 s) where the pressure is constant and is imposed by the upstream reservoir.

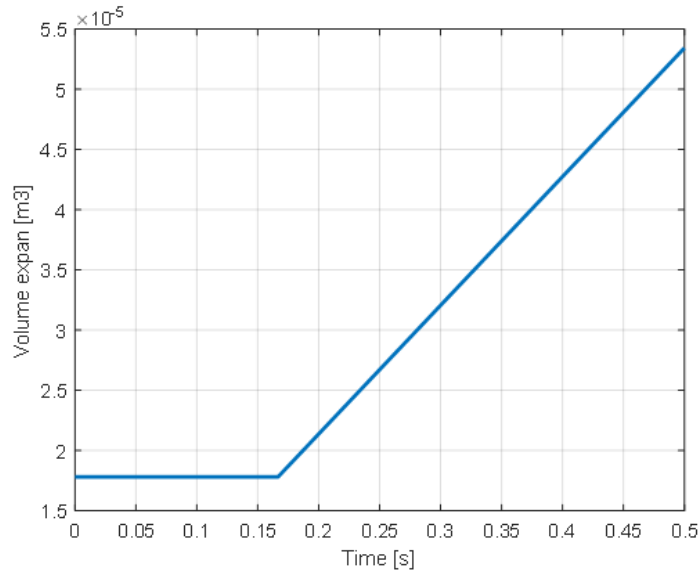


Fig. 18: Volume of expansion.

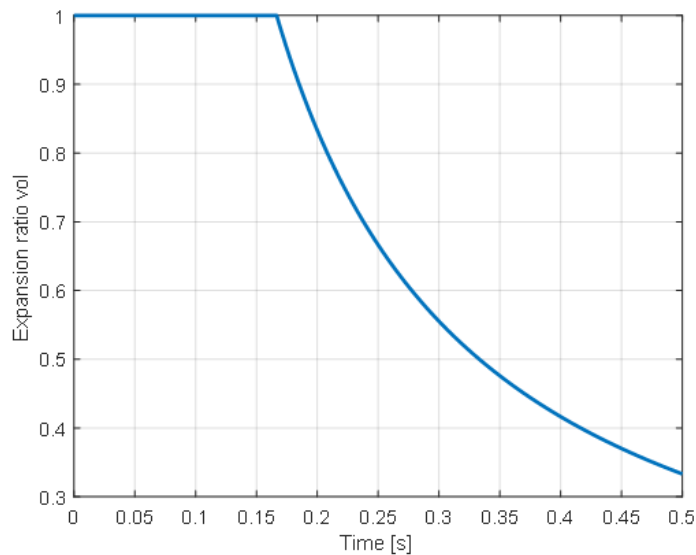


Fig. 19: Volume ratio of the expansion)

**2.3.2 Mass of the intaken gas**

The evolution of the pressure and of the temperature during expansion can be calculated with the classic relations given in rel. (3) and (14). In that relations only the variation of the volume is considered and the nature or the mass of the gas does not appear in the expressions. But for the use of a more accurate model as the Van der Waals or the Beattie Bridgeman model the mass volume  $v$  or the molar volume  $\bar{v}$  must be known. The relation of these variables to the

mass of gas is given through:

$$v = \frac{V}{m} \quad \text{and} \quad \bar{v} = M \cdot v = M \cdot V / m \tag{18}$$

The volume  $V$  and the pressure  $P$  are given but the mass  $m$  must be evaluated. A first approach uses the ideal gas law and gives in this case:

$$m = \frac{P \cdot V}{R \cdot T} = \frac{160 \cdot 10^3 \text{ N/m}^2 \cdot 53.5 \cdot 10^{-6} \text{ m}^3 \cdot \frac{1}{3}}{4.124 \text{ kJ/kg} \cdot \text{K}^{-1} \cdot 293 \text{ K}} = 2.361 \cdot 10^{-4} \text{ kg} \tag{19}$$

Considering the use of the Van der Waals model, and the initial conditions  $P$  and  $V$  before the expansion, the

temperature of the gas can be calculated with rel. (20) and should correspond to the atmospheric temperature.



$$T = \frac{\left(P + \frac{a}{v^2}\right)}{R} (v - b) \tag{20}$$

From rel. (7) and with the values of Table 1 the factors a and b become

$$a = \frac{27R^2 \cdot T_{cr}^2}{64P_{cr}} = \frac{27 \cdot (4.124 \cdot \text{kJ} / \text{kgK})^2 \cdot (33.3\text{K})^2}{64 \cdot 1.3\text{MPa}} = 6.120\text{kPa} \cdot \text{m}^6 / \text{kg}^2 \tag{21}$$

$$b = \frac{R \cdot T_{cr}}{8P_{cr}} = \frac{4.124\text{kJ} / \text{kgK} \cdot 33.3\text{K}}{8 \cdot 1.3\text{MPa}} = 0.0132\text{m}^3 / \text{kg} \tag{22}$$

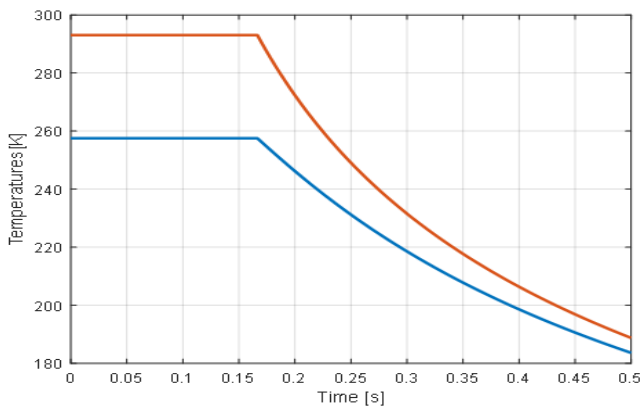
Still in the situation of constant pressure before the expansion the mass volume is

$$v = \frac{V}{m} = \frac{53.5 \cdot 10^{-6} \text{m}^3 / 3}{2.361 \cdot 10^{-4} \text{kg}} = 0.0755\text{m}^3 / \text{kg} \tag{23}$$

The temperature calculated with the Van der Waals model based on this value of the mass volume  $v$  being:

$$T = \frac{\left(P + \frac{a}{v^2}\right)}{R} (v - b) = \frac{160 \cdot 10^5 \text{N} / \text{m}^2 + (6.120\text{kPa} \cdot \text{m}^6 / \text{kg}^2) / (0.0755\text{m}^3 / \text{kg})^2}{4.124\text{kJ} / \text{kgK}} \cdot (0.0755\text{m}^3 / \text{kg} - 0.0132\text{m}^3 / \text{kg}) = 257.5\text{K} \tag{24}$$

This value does not correspond to the temperature of the intaken gas and shows the difference between the ideal gas model and the Van der Waals model, especially for high pressures. Fig. 20 shows the difference between the two models. During the filling with constant pressure (0 – 0.166s) the difference of the temperature is significant (257.5K instead of 293K) because of the chosen value of the gas mass. A right modeling of the temperature should include the real value of the gas mass. Consequently, the value of the mass volume should be calculated using rel. (20) with imposed pressure and temperature. The form of this relation however does not allow a resolution versus  $v$  and needs another method for the evaluation of the right value of the gas mass in the cylinder.



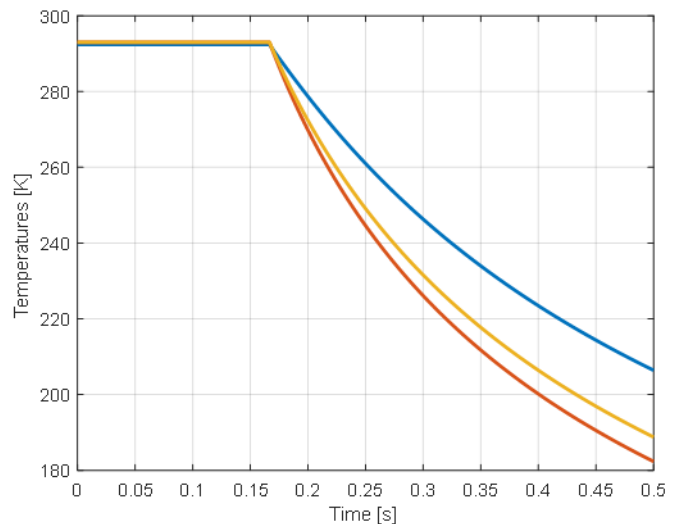
**Fig. 20:** Evolution of the temperature calculated with the ideal gas law (red) and with the not corrected Van der Waals model (blue)

In the present study an iterative method based on the simulation of rel. (20) is used and leads to a corrected value of the mass of  $2.1 \cdot 10^{-4} \text{kg}$  of Hydrogen instead of the  $2.361 \cdot 10^{-4} \text{kg}$  calculated previously.

### 2.3.3 Simulation of the expansion

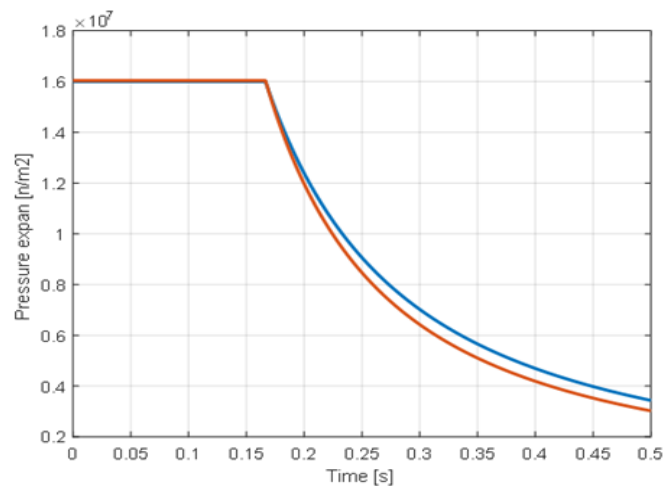
Figure 21 shows three different evaluations of the temperature with three different models, namely the ideal gas law (yellow), a Van der Waals model (with corrected value of the gas mass) where the evolution of the pressure is calculated with the ideal gas law (blue), and a Van der Waals model completed with integrated thermal model (TIM), (red curve).

The structural diagram of the TIM model used here for the expansion is identical to the model represented in Fig. 12 and previously used for compression.



**Fig. 21:** Evolution of the temperature with the ideal gas law (yellow), Van der Waals with idealized pressure (blue) and Van der Waals with TIM model (red).

The Van der Waals TIM model of Fig. 12 does not only represent the evolution of the temperature but gives also the evolution of the pressure (Fig. 22).



**Fig. 22:** Pressure of expansion in adiabatic mode with VDW TIM (blue) and ideal gas law (red).

### 3. Discussion

The state equations used in the simulation of compression of air and hydrogen have been implemented in simulations where the mechanical variables as the volumetric ratio is imposed. The different models bring similar results especially in the isothermal mode and when the pressure is not going above the values of 50 to 100 bar. For the simulation of the variation of the temperature, an easy-to-implement thermal model (TIM, Thermal Integrated Model) is used where the energy corresponding to transferred mechanical work to the gas is considered. The thermal model is inserted “in-the-loop” with the functional diagrams representing the state equations. Regarding the results of simulations only small differences are observed in the order of a few percent. In the present study only the adiabatic mode is simulated, but any polytropic phenomena can be represented with the TIM model as long as the thermal resistance between compressed gas and the surrounding would be known.

For the simulation of the expansion mode the same models are used. One larger difference is observed in relation to the considered mass of gas which is initially in the volume to be expanded. The estimation of that mass in dependency of the initial pressure and temperature and from the state equations has been realized by successive iterations by variation of the factor representing the mass volume  $v$ . For the simulation of the temperature a comparison is made between the ideal gas law model and the Van der Waals model in open loop and where the pressure is calculated with the analytic relation. A further comparison is made with the Van der Waals model completed by the TIM model. The results show differences in the order of 10 to 15 percent.

For the representation of the variation of the pressure in expansion mode the comparison is made between the ideal gas law and the completed TIM model. Only small differences are observed in the range of 3 to 5 percent. Detailed informations on the differences between the used state equations for the present study can be found in reference [10].

### 4. Conclusions

The present study sets in evidence the differences in using different formulations for the representation of the variation of pressure and temperature of a non-ideal gas like hydrogen during compression and expansion in a cylinder where the

volumetric ratio is varied. The differences observed in the curves of temperature and pressure must be considered as relevant for the estimation of the real behavior of the thermodynamic processes, but an accurate model for the representation of the thermal flow exchanged from the compressed gas to the surrounding should be used. Indeed, the largest differences observed in the simulations are related to the considered characteristics between isothermal and adiabatic curves and illustrates the importance to know better the amount of exchanged heat from the gas to the surrounding.

The effect of the compression pressure on the effort to be spent by the external force is another theme that should be considered and completed by a model which should include the mechanical friction. Friction forces of the high-pressure seals are easy to estimate by experimental measures without pressure produced (open valves), but their correct estimation under high pressure is quasi-impossible. Only indirect method could bring answer by calculation of the difference between measured force and calculated pressure-related force.

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