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Engine Control System Development and Symbolic Manipulation
- Application and Challenges in Modelling -

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Abstract

The integrated use of symbolic and numeric technologies is presented through application examples in automotive industry. The effectiveness of such an integrated approach is emphasized by showing concrete uses of symbolic manipulation and numerical computation in Maple [1]. In the first of the two examples, the chemical equilibrium of combustion phenomena which is a constrained optimization problem is analysed symbolically and turned into an unconstrained optimization problem. As opposed to numeric-only approach, target equations for the minimization problem are explicitly shown, which facilitates the understanding of the problem. In the second example, a simple phenomenological model for the heat release process of an internal combustion engine is introduced where a differential equation containing a conditional branch is symbolically analysed and then numerically integrated to obtain some key physical quantities of the combustion dynamics. Finally, the paper is concluded with some remarks on challenges that modelling technologies in automotive industry are facing.

Introduction

Today, there are about 800 million vehicles including passenger cars, trucks and buses worldwide and the number is still growing rapidly, particularly in emerging countries such as China and India [2]. While the new types of power sources for a vehicle, notably hybrid electric, are increasingly becoming popular in some countries, the vast majority of new vehicles produced and sold today come with an internal combustion engine only, and this trend may be attributed to various facts such as 1) the balance between the income level of individual households and the price range of vehicles, or 2) the car ownership rate in each country and people's appetite for buying expensive goods including a car. Because of the constant increase in the number of engines operating at every corner of the cities around the world, the amount of exhaust emissions from vehicles is also increasing, and thus regulations on emissions are under constant revisions to get more stringent.

On this backdrop, the control system of an engine of a vehicle has grown in its complexity with more actuators and sensors, and/or more precise control than ever before. This trend has necessitated the front-loading in a development process, and the use of models (generally called "plant models") of engines and other vehicle components such as transmission or battery at an early stage of a development process (commonly called "Model-Based Development" or acronymed MBD), has become the norm in automotive industry. Although the hitherto effort for the front-loaded development is enabling ever more efficient development, still more effort is required as the complexity of the control system keeps growing.

In order to meet increasingly demanding requirements on plant models, new technologies for modelling and simulation of a physical system are gaining a foothold (for example Modelica [3], VHDL-AMS [4] and Simscape [5]). These technologies provide important features like automatic physical equation generation for component connections and DAE solvers for a hybrid system, and are playing a key role in the system level simulation. However, capturing the physics behind a system in question is out of scope of these technologies, i.e., the authors of physical component models must take responsibility of the equations that they derive and define. Today, this equation-derivation process for a physical component is considered a task with paper and a pen or some word-processing software, but the productivity of this process needs to increase so that essential physical phenomena can be modelled in a timely manner and used efficiently as part of a system for fully fledged system level simulations. As an attempt to fill this gap, in this article the author would like to propose to use symbolic manipulation technology together with numerical computation technology and show how the equational analysis process can be streamlined.

This paper is organized as follows. First, the combustion chemistry is analysed symbolically so that the problem can be presented as an unconstrained optimization problem. Second, the phenomenological heat release process in an internal combustion engine is analysed and numerically integrated. Through these two cases, the potential benefit of the integrated use of symbolic and numeric approaches will be exposed. Finally, the paper is concluded with some brief remarks on other issues not dealt in the paper.

This paper itself is a Maple worksheet where the symbolic and numeric operations appearing below are computationally processed. The version of Maple being used is as follows.

Standard Worksheet Interface, Maple 17.00, Windows 7, April 10 2013 Build ID 827314 **(1)**

Modelling Example 1 - Combustion Chemistry & Chemical Equilibrium

Background

In an internal combustion engine of a vehicle, combustion is repeatedly occurring several thousand times at every minute. For example, suppose an engine is running at 1000 or 6000 revolutions per minute (RPM), then a single revolution of an engine crank takes just 60 or 10 milliseconds, respectively. A combustion of the mixture of air and fuel vapour (and, strictly speaking, some residual burned gas too) is controlled in terms of the air-to-fuel ratio and the combustion start timing. At every combustion phenomenon, fuel vapour of about 10 to 20 milligrams is burned to generate torque which drives the wheels. At the same time, the water and carbon dioxide, together with other various kinds of molecules depending on operating conditions, are produced.

In the case of combustion at stoichiometry where both the air and the fuel are completely consumed, the chemical reaction formula is described as follows [6].

$$C_8H_{18} + 12.5\left(\mathrm{O}_2 + 3.773\,N_2\right) = 9\,H_2\mathrm{O} + 8\,CO_2 + 47.16\,N_2$$

where the fuel is assumed octane. In general, however, the combustion reaction in an internal combustion engine can never occur at stoichiometry because of various kinds of disturbances such as variances in fuel injection amount, thermal exchange with cylinder wall or piston action and so on. Considering these effects, the reaction may be generally represented as follows [8].

$$\frac{\phi}{a + \frac{b}{4} - \frac{c}{2}}\,C_aH_b\mathrm{O}_c + \mathrm{O}_2 + 3.773\,N_2 = x_1H_2\mathrm{O} + x_2CO_2 + x_3N_2 + \ldots$$

The last term on the R.H.S. of the above equation (...) indicates species such as NOx, CO, OH, H etc. whose production depends on operating conditions, and ϕ is the fuel-to-air equivalence ratio. Regardless of the product types, the element mass involved in the reaction must conserve.

$$\sum_{j=1}^{n}\left(A_{ij}n_j - \beta_i\right) = 0 \qquad \textbf{(2)}$$

where A_{ij} are the stoichiometric coefficients, n_j is the number of moles of product species j, β_i is the number of moles of element $i = C, H, \mathrm{O}, N$ for 1 mole of oxygen in the air. Specifically, β_i for each element can be defined based on the above general reaction formula as follows.

$$\beta_C = \frac{a\,\phi}{a + \frac{1}{4}b - \frac{1}{2}c},\ \beta_H = \frac{b\,\phi}{a + \frac{1}{4}b - \frac{1}{2}c},\ \beta_{\mathrm{O}} = 2 + \frac{c\,\phi}{a + \frac{1}{4}b - \frac{1}{2}c},\ \beta_N = 7.546 \qquad \textbf{(3)}$$

According to [6], "it is a good approximation for performance estimates in engines to regard the burned gases produced by the combustion of fuel and air as in chemical equilibrium" excluding the late expansion stroke and during the exhaust process. Chemical equilibrium is achieved when the Gibbs free energy of a mixture

$$g = \sum_{j=1}^{n} g_{mole_j}\,n_j \qquad \textbf{(4)}$$

is minimized where g_{mole_j} denotes the Gibbs free energy (or equivalently the chemical potential) of species j per mole. For gases, the chemical potential g_{mole_j} is

$$g_{mole_j}\left(x_j, p, T\right) = g_{p,mole_j}(T) + R_{univ}T\ln\left(x_j\right) + R_{univ}T\ln\left(\frac{p}{p0}\right) \qquad \textbf{(5)}$$

where $g_{p,mole_j}$ is the chemical potential in the standard state, x_j is the mole fraction of species j, p is the pressure of the gas, T is the temperature of the gas, and $p0$ is the reference pressure. The mole fraction x_j is defined as follows.

$$x_j = \frac{n_j}{n_{tot}} \qquad \textbf{(6)}$$

where n_{tot} is the sum of the number of moles of all product species.

Several methods to minimize the Gibbs free energy g were proposed in literatures [6], [7], [8]. One way in [6] is to use the method of Lagrange multipliers λ_i and the equilibrium conditions are given as

$$g_{mole_j}\left(x_j, p, T\right) + \sum_{i=1}^{l} \lambda_i A_{i,j} = 0 \tag{7}$$

So far, the explanations were kept as general as possible. Now, concrete calculations are going to be performed step by step so that this problem can better be exposed for a specific case.

Example

Definitions of Basic Quantities

First, the fuel is assumed to be iso-octane C_8H_{18}

$$fuel\_params := [a = 8, b = 18, c = 0] \tag{8}$$

and the following product species are assumed

$$species := [H2O, CO2, N2, O2, CO, NO, OH, H, H2, \mathrm{O}] \tag{9}$$

The elements included in the reaction are as follows.

$$elements := [C, H, \mathrm{O}, N] \tag{10}$$

Then A_{ij}, n_j and β_i are determined.

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 0 \\ 1 & 2 & 0 & 2 & 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{11}$$

$$n^T = \begin{bmatrix} n_{H2O} & n_{CO2} & n_{N2} & n_{O2} & n_{CO} & n_{NO} & n_{OH} & n_{H} & n_{H2} & n_{\mathrm{O}} \end{bmatrix} \tag{12}$$

$$\beta^T = \begin{bmatrix} \frac{16}{25}\phi & \frac{36}{25}\phi & 2 & 7.546 \end{bmatrix} \tag{13}$$

Note that the fuel/air equivalence ratio ϕ is kept as symbol for β_i as it varies in every combustion cycle.

Element Conservations

Now the element conservations, Eq.**(2)**, can be written in a concrete manner.

$$\begin{gathered} n_{CO2} + n_{CO} - \frac{16}{25}\phi = 0 \\ 2\,n_{H2O} + n_{OH} + n_{H} + 2\,n_{H2} - \frac{36}{25}\phi = 0 \\ n_{H2O} + 2\,n_{CO2} + 2\,n_{O2} + n_{CO} + n_{NO} + n_{OH} + n_{\mathrm{O}} - 2 = 0 \\ 2\,n_{N2} + n_{NO} - 7.546 = 0 \end{gathered} \tag{14}$$

where the fuel-to-air equivalence ratio ϕ is a parameter that is determined at every combustion cycle through fuel injection.

Note that understanding the physical meanings of the above equations is facilitated thanks to physically meaningful subscripts such as *CO2* or *OH* etc. instead of integers while the use of the symbolic manipulation software package maintains the possibility to apply manipulations on these equations efficiently.

Chemical Potential & Lagrange Multipliers for Minimization

Similar to the mass conservation equations, Eq.**(7)** can also be made specific for the current case.

First, all the subscripts are made specific. Here, only three equations out of ten are shown to save the space.

$$\begin{gathered} g_{moleH2O}\left(x_{H2O}, p, T\right) + \lambda_1 A_{1,1} + \lambda_2 A_{2,1} + \lambda_3 A_{3,1} + \lambda_4 A_{4,1} = 0 \\ g_{moleCO2}\left(x_{CO2}, p, T\right) + \lambda_1 A_{1,2} + \lambda_2 A_{2,2} + \lambda_3 A_{3,2} + \lambda_4 A_{4,2} = 0 \end{gathered} \tag{15}$$

$$g_{mole_{N2}}\left(x_{N2}, p, T\right) + \lambda_1 A_{1,3} + \lambda_2 A_{2,3} + \lambda_3 A_{3,3} + \lambda_4 A_{4,3} = 0 \tag{15}$$

Then the matrix A_{ij} is substituted, and the subscripts for λ_i are replaced from integers to element symbols.

$$\begin{gathered}
g_{mole_{H2O}}\left(x_{H2O}, p, T\right) + 2\lambda_H + \lambda_O = 0 \\
g_{mole_{CO2}}\left(x_{CO2}, p, T\right) + \lambda_C + 2\lambda_O = 0 \\
g_{mole_{N2}}\left(x_{N2}, p, T\right) + 2\lambda_N = 0 \\
g_{mole_{O2}}\left(x_{O2}, p, T\right) + 2\lambda_O = 0 \\
g_{mole_{CO}}\left(x_{CO}, p, T\right) + \lambda_C + \lambda_O = 0 \\
g_{mole_{NO}}\left(x_{NO}, p, T\right) + \lambda_O + \lambda_N = 0 \\
g_{mole_{OH}}\left(x_{OH}, p, T\right) + \lambda_H + \lambda_O = 0 \\
g_{mole_{H}}\left(x_{H}, p, T\right) + \lambda_H = 0 \\
g_{mole_{H2}}\left(x_{H2}, p, T\right) + 2\lambda_H = 0 \\
g_{mole_{O}}\left(x_{O}, p, T\right) + \lambda_O = 0
\end{gathered} \tag{16}$$

These equations are part of the target equations for minimization.

Now the first term on the L.H.S. of Eq.**(16)**, which is the Gibbs free energy of each species defined in Eq.**(5)**, needs to be computed. In Eq.**(5)**, the first term on the R.H.S. is the chemical potential in the standard state $g_{p,mole_j}(T)$ and can be computed as follows. First, the chemical potential is related to other thermodynamic quantities as

$$g_{p,mole_j}(T) = h_{mole_j}(T) - T s_{p,mole_j}(T) \tag{17}$$

where h_{mole_j} and $s_{p,mole_j}$ are the enthalpy and the entropy of species j per mole in the standard state, respectively. These quantities can be computed from the following polynomials.

$$\begin{aligned}
\frac{h_{mole_j}(T)}{R_{univ} T} &= a_{1_j} + \frac{1}{2} a_{2_j} T + \frac{1}{3} a_{3_j} T^2 + \frac{1}{4} a_{4_j} T^3 + \frac{1}{5} a_{5_j} T^4 \\
\frac{s_{p,mole_j}(T)}{R_{univ}} &= a_{1_j} \ln(T) + a_{2_j} T + \frac{1}{2} a_{3_j} T^2 + \frac{1}{3} a_{4_j} T^3 + \frac{1}{4} a_{5_j} T^4 + a_{7_j}
\end{aligned} \tag{18}$$

where $R_{univ} = 8.3143$ (J/mol/K) is the universal gas constant, and the coefficients on the R.H.S. a_{k_j} ($k = 1 ..7$) are known values for various kinds of molecules and publicly available as a data table released as GRI-Mech [9]. The polynomials for enthalpy and entropy were derived from the one for specific heat $c_{p,mole_j}$, and these are called the NASA polynomials [8].

$$\frac{c_{p,mole_j}(T)}{R_{univ}} = T^4 a_{5_j} + T^3 a_{4_j} + T^2 a_{3_j} + T a_{2_j} + a_{1_j} \tag{19}$$

The values of the coefficients for each species consist of two different groups below and above a threshold temperature. For example, the values for NO are

$T1 = 1000.0$, $a_{hi_1} = 3.2606056$, $a_{hi_2} = 0.0011911043$, $a_{hi_3} = -4.2917048\ 10^{-7}$, $a_{hi_4} = 6.9457669\ 10^{-11}$, $a_{hi_5} = -4.0336099\ 10^{-15}$, $a_{hi_6} = 9920.9746$, $a_{hi_7} = 6.3693027$, $a_{low_1} = 4.2184763$, $a_{low_2} = -0.0046389760$, $a_{low_3} = 0.000011041022$, $a_{low_4} = -9.3361354\ 10^{-9}$, $a_{low_5} = 2.8035770\ 10^{-12}$, $a_{low_6} = 9844.6230$, $a_{low_7} = 2.2808464$ **(20)**

where $T1$ is the threshold temperature in Kelvin, a_{hi_k} and a_{low_k} ($k = 1 ..7$) are the values above and below that threshold, respectively.

Now all the necessary equations were presented. Eqs.**(17)** and **(5)** are going to be computed for each species.

As an example, the Gibbs free energy of *H2O* in the standard state looks as follows. Below the threshold temperature of 1000 K,

$$g_{p,mole_{H2O}}(T) = 8.3143\,T\,(5.047672768 + 0.001018217050\,T - 0.000001086733685\,T^2 + 4.57330885\,10^{-10}\,T^3 - 8.85989085\,10^{-14}\,T^4 - 4.19864056\ln(T)) \tag{21}$$

Above the threshold temperature,

$$g_{p,mole_{H2O}}(T) = 8.3143\,T\,(-1.932777610 - 0.001088459020\,T + 2.734541967\,10^{-8}\,T^2 + 8.08683225\,10^{-12}\,T^3 - 8.41004960\,10^{-16}\,T^4 - 3.03399249\ln(T)) \tag{22}$$

The complete Gibbs free energy of *H2O* as a function of the mole fraction, pressure and temperature is

$$g_{mole_{H2O}}(x_{H2O}, p, T) = g_{p,mole_{H2O}}(T) + 8.3143\,T\ln(x_{H2O}) + 8.3143\,T\ln(0.000009869232667\,p) \tag{23}$$

Similar calculations can be performed for the other species. By substituting Eq.**(23)** and similar equations for the other species into Eqs.**(16)**, ten equations with 14 unknowns (ten mole fractions x_j and four Lagrange multipliers λ_i) and 2 parameters (i.e., pressure p and temperature T) are obtained. Four more equations are mass conservation equations Eq.**(14)**.

The mole fraction x_j and the number of moles n_j are related through Eq.**(6)** where the total number of moles n_{tot} can be specifically described for the current case as

$$n_{tot} = n_{H2O} + n_{CO2} + n_{N2} + n_{O2} + n_{CO} + n_{NO} + n_{OH} + n_{H} + n_{H2} + n_{\mathrm{O}} \tag{24}$$

Unconstrained Optimization Problem

The equations **(14)**, **(16)**, **(24)**, together with **(21)**, **(22)**, **(23)** and similar equations for the other species, constitute the set of equations to solve. Note that some operating conditions need to be specified. Specifically, in Eq.**(23)**, pressure p and temperature T must be specified. In Eq.**(14)**, equivalence ratio ϕ needs to be specified. The target variables for the minimization are n_j. The mole fractions x_j are basically the same as n_j except that they are normalized by n_{tot}.

In the spirit of seeing is believing, let us see the final set of equations for minimization by specifying all the remaining parameter values. This can be very easily performed here because this article is in fact a Maple worksheet where all the manipulations and calculations so far were carried out in Maple.

When the conditions are

$$p = 2.026500\,10^5,\ T = 2000,\ \phi = 1.0 \tag{25}$$

the equations are

$$\begin{gathered}
-4.376150190\,10^5 + 16628.6000\ln(x_{H2O}) + 2.\,\lambda_H + \lambda_{\mathrm{O}} = 0. \\
-5.036846888\,10^5 + 16628.6000\ln(x_{CO2}) + \lambda_C + 2.\,\lambda_{\mathrm{O}} = 0. \\
-4.286312600\,10^5 + 16628.6000\ln(x_{N2}) + 2.\,\lambda_N = 0. \\
-4.577501428\,10^5 + 16628.6000\ln(x_{O2}) + 2.\,\lambda_{\mathrm{O}} = 0. \\
-4.420203868\,10^5 + 16628.6000\ln(x_{CO}) + \lambda_C + \lambda_{\mathrm{O}} = 0. \\
-4.680479299\,10^5 + 16628.6000\ln(x_{NO}) + \lambda_{\mathrm{O}} + \lambda_N = 0. \\
-4.121053883\,10^5 + 16628.6000\ln(x_{OH}) + \lambda_H + \lambda_{\mathrm{O}} = 0. \\
-2.554556388\,10^5 + 16628.6000\ln(x_H) + \lambda_H = 0. \\
-3.044823405\,10^5 + 16628.6000\ln(x_{H2}) + 2.\,\lambda_H = 0. \\
-3.490007755\,10^5 + 16628.6000\ln(x_{\mathrm{O}}) + \lambda_{\mathrm{O}} = 0. \\
n_{CO2} + n_{CO} - 0.6400000000 = 0. \\
2.\,n_{H2O} + n_{OH} + n_H + 2.\,n_{H2} - 1.440000000 = 0. \\
n_{H2O} + 2.\,n_{CO2} + 2.\,n_{O2} + n_{CO} + n_{NO} + n_{OH} + n_{\mathrm{O}} - 2. = 0. \\
2.\,n_{N2} + n_{NO} - 7.546 = 0.
\end{gathered} \tag{26}$$

When the conditions are

$$p = 1.0132500\,10^6,\ T = 2500,\ \phi = 0.5 \tag{27}$$

the equations are

$$\begin{gathered}
-5.367924725\,10^5 + 20785.7500\ln\left(x_{H2O}\right) + 2.\,\lambda_H + \lambda_O = 0. \\
-6.255020045\,10^5 + 20785.7500\ln\left(x_{CO2}\right) + \lambda_C + 2.\,\lambda_O = 0. \\
-5.203828734\,10^5 + 20785.7500\ln\left(x_{N2}\right) + 2.\,\lambda_N = 0. \\
-5.580052376\,10^5 + 20785.7500\ln\left(x_{O2}\right) + 2.\,\lambda_O = 0. \\
-5.371483275\,10^5 + 20785.7500\ln\left(x_{CO}\right) + \lambda_C + \lambda_O = 0. \\
-5.703948517\,10^5 + 20785.7500\ln\left(x_{NO}\right) + \lambda_O + \lambda_N = 0. \\
-4.989796192\,10^5 + 20785.7500\ln\left(x_{OH}\right) + \lambda_H + \lambda_O = 0. \\
-2.974616894\,10^5 + 20785.7500\ln\left(x_H\right) + \lambda_H = 0. \\
-3.643732573\,10^5 + 20785.7500\ln\left(x_{H2}\right) + 2.\,\lambda_H = 0. \\
-4.144924437\,10^5 + 20785.7500\ln\left(x_O\right) + \lambda_O = 0. \\
n_{CO2} + n_{CO} - 0.3200000000 = 0. \\
2.\,n_{H2O} + n_{OH} + n_H + 2.\,n_{H2} - 0.7200000000 = 0. \\
n_{H2O} + 2.\,n_{CO2} + 2.\,n_{O2} + n_{CO} + n_{NO} + n_{OH} + n_O - 2. = 0. \\
2.\,n_{N2} + n_{NO} - 7.546 = 0.
\end{gathered} \tag{28}$$

There already exist many solution methods and implementations for this type of problem, but the real challenge of this problem from the standpoint of the development of an engine control system is not simply to choose an optimization method. Rather, the challenges are 1) the above optimization problem must be solved many times - actual phenomenon are repeated several thousand times per minute - with different initial conditions for the fuel-to-air ratio, pressure and temperature for every combustion cycle, 2) the gas pressure and temperature are affected by, not only the combustion, but also the piston action as well as thermal energy exchange between the gas and the cylinder wall, 3) the combustion phenomena is just one of many dynamics occurring in an engine, all of which must be computed as a system, 4) an engine plant model needs to be connected with an engine controller, which may be a model or a real control unit, to form a closed-loop system, 5) such a closed-loop simulation needs to run at a reasonable speed and 6) more and more precise calculations will be required in future as the regulations on the emissions become tighter and tighter.

Although there are some dedicated simulation packages for combustion chemistry, it is difficult to meet these challenges with them as they usually are not designed to be integrated as part of an entire engine model, which has to be further integrated with (a) controller(s).

With the symbolic manipulation technology, seemingly complicated problems like combustion chemistry may be understood and grappled with efficiently as presented above. Furthermore, it would be very productive if "code" to solve the optimization problem can be directly produced for a target simulation environment from the symbolic-numeric analysis. In such a case, the code may not necessarily be C or other procedural programming languages. Rather, it may be a plant modelling language such as Modelica or Simscape so that the code can be used as part of an entire engine model implemented in that target environment.

Modelling Example 2 - Combustion Dynamics in Internal Combustion Engines

In the previous section, a single combustion phenomenon was examined. However, as mentioned previously, real engine cycle involves several thousand combustion phenomena at every minute. During each cycle, a piston and valves work together to inhale and compress the gas which is then burned and presses down the piston for work and is exhaled from the cylinder. In this section, a phenomenological heat release model for this engine cycle is introduced. As opposed to the previous example where the system was algebraic, the system of this example consists of a differential equation containing a conditional branch, and it will be shown that the symbolic manipulation technology works well for this type of system when it is used in conjunction with numerical computation technology.

First, model parameters are defined, but the detailed explanations for each parameter is omitted and some are going to be explained later as needed. Here, a single-cylinder engine is assumed to be operating at a constant speed of $\omega_{eng} = 40\,\pi$ (rad/s) = 1200 (RPM).

$$\overset{33\ parameters}{\Big[p_{amb} = 101325,\ l_{bore} = 0.081,\ l_{stroke} = 0.077,\ l_{rod} = 0.122,\ s_{tdc} = 0.008500000000,\ l_{crk} = 0.03850000000,\ A_{cyl} = 0.005152997351,\ V_{clear} = 0.00004380047748,\ V_{disp} = 0.0004405812735,\ f_{air} = 5,\ R_{air} = 287,\ Cv_{air} = \frac{1435}{2},\ H_{low} = 4.25\ 10^{7},\ T0 = 293.15,\ P0 = 101325,\ V0 = 0.0004405812735,\ m_{air} = 0.0002122417620,\ e_{ini} = 44.64189754,\ KL = 0.4,\ AFR = 14.6,\ SA_{deg} = 15,\ RPM = 1200,\ T_{wall} = 373.15,\ k_{therm} = \frac{2}{5},\ SA_{rad} = 2.879793266,\ m_{fuel} = 0.00001453710699,\ Q_{\max} = 617.8270471,\ \omega_{eng} = 40\,\pi,\ c_1 = 1.2,\ c_2 = 500,\ c_3 = 0.000001,\ a_{wi} = 6.907755279,\ m_{wi} = 3\Big]} \tag{29}$$

Piston position z_{piston} as a function of crank angle θ_{rad} can be calculated by

$$z_{piston}(\theta_{rad}) = l_{stroke} - l_{crk}\,(1 - \cos(\theta_{rad})) - l_{rod}\left(1 - \sqrt{1 - \frac{\sin(\theta_{rad})^2\, l_{crk}^2}{l_{rod}^2}}\right) \tag{30}$$

where l_{stroke}, l_{rod}, l_{crk} are the lengths of piston stroke, connecting-rod and crank, respectively.

Using Eq.**(30)**, the volume of a cylinder is readily computed as

$$V_{cyl}(\theta_{rad}) = V_{clear} + A_{cyl}\, z_{piston}(\theta_{rad}) \tag{31}$$

where V_{clear} is the clearance volume and A_{cyl} is the area of a piston head. This will be used when thermodynamic quantities of the gas are calculated.

Thermodynamics of ideal gas in a cylinder

According to thermodynamics, internal energy of ideal gas e_{cyl} is given by

$$e_{cyl}(\theta_{rad}) = \frac{1}{2} f_{air}\, p_{cyl}(\theta_{rad})\, V_{cyl}(\theta_{rad}) \tag{32}$$

where f_{air} is the degrees of freedom of air molecule. Also, the ideal gas law states

$$p_{cyl}(\theta_{rad})\, V_{cyl}(\theta_{rad}) = m_{air}\, R_{air}\, T_{cyl}(\theta_{rad}) \tag{33}$$

where m_{air} is the mass of air in the cylinder and R_{air} is the specific gas constant of air. It should be noted that the use of parameters for air is approximation since the actual gas in the cylinder is a mixture of air, fuel vapour and residual burned gas and their composition varies as combustion reaction progresses.

Eq.**(32)** can be rearranged so that the gas pressure can be calculated from the internal energy.

$$p_{cyl}(\theta_{rad}) = \frac{2\, e_{cyl}(\theta_{rad})}{f_{air}\, V_{cyl}(\theta_{rad})} \tag{34}$$

Note that the cylinder volume V_{cyl} can be calculated from Eq.**(31)**.

From Eqs.**(32)** and **(33)**, the gas temperature can also be calculated from the internal energy.

$$T_{cyl}(\theta_{rad}) = \frac{2\, e_{cyl}(\theta_{rad})}{f_{air}\, m_{air}\, R_{air}} \qquad \textbf{(35)}$$

In the remainder of this section, the dynamics of the internal energy of the gas during compression and expansion strokes will be modelled as a differential equation. So, let us first clarify the initial condition, which can be determined from Eq.**(32)**.

$$e_{cyl}(0) = 44.64189754 \qquad \textbf{(36)}$$

Adiabatic Motoring

For the sake of better comprehension of the problem, the simplest case of the gas dynamics in a closed volume with a moving piston is considered first.

When a piston is moving but there is no combustion (i.e. so-called "motoring") as well as no thermal energy exchange between the gas and the cylinder wall (i.e. adiabatic), the change in the internal energy of the gas is caused by the piston work only.

$$\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}}\, e_{cyl}(\theta_{rad}) = -p_{cyl}(\theta_{rad}) \left(\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}}\, V_{cyl}(\theta_{rad}) \right) \qquad \textbf{(37)}$$

The R.H.S. of the above equation can be computed from Eq.**(34)** for the pressure and Eq.**(31)** for the cylinder volume.

Adiabatic Combustion

Now let us consider combustion. (Thermal exchange is not considered yet.) To deal with combustion phenomenon of an engine, there are many models proposed over the past decades. In this article, a phonomenological model often used for analyzing basic thermodynamics of combustion, called Wiebe heat-release model [6], is going to be employed. This model can estimate the heat release due to the combustion of fuel and air during an engine cycle with relatively small number of empirical model parameters, and is suitable for cycle-by-cycle torque estimation. Here, Wiebe model will be defined, analysed and simulated using both symbolic and numeric approaches.

Wiebe model needs another submodel for burn duration estimation, which is given in this article as a function of the engine speed.

$$\theta_{bd}(\omega_{eng}) = \frac{c_1\, \omega_{eng}}{c_2} - c_3\, \omega_{eng}^2 \qquad \textbf{(38)}$$

where c_i (i = 1, 2, 3) need to be adjusted to experimental data.

Wiebe heat-release model itself is given as follows.

$$x_{burn}(\theta_{rad}) = \begin{cases} 0 & \theta_{rad} \le SA_{rad} \\ 1 - \mathrm{e}^{-a_{wi} \left(\frac{\theta_{rad} - SA_{rad}}{\theta_{bd}(\omega_{eng})} \right)^{m_{wi}+1}} & \textit{otherwise} \end{cases} \qquad \textbf{(39)}$$

where SA_{rad} is spark angle (or start of combustion) which is a control signal, a_{wi} and m_{wi} are adjustable parameters. For your information, the equation looks as follows when parameter values are substituted.

$$x_{burn}(\theta_{rad}) = \begin{cases} 0. & \theta_{rad} \le 2.879793266 \\ 1. - 1.\,\mathrm{e}^{-1035.329906\, (\theta_{rad} - 2.879793266)^4} & \textit{otherwise} \end{cases} \qquad \textbf{(40)}$$

This helps understand that this heat-release model returns 0 prior to the combustion, and that once the combustion starts at SA_{rad}, the value increases until it reaches 1 which corresponds to the end of combustion.

Heat release rate can be derived from Wiebe function.

$$\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}}\, x_{burn}(\theta_{rad}) = \begin{cases} 0 & \theta_{rad} \le SA_{rad} \\ \dfrac{a_{wi} \left(\dfrac{\theta_{rad} - SA_{rad}}{\theta_{bd}(\omega_{eng})} \right)^{m_{wi}+1} (m_{wi} + 1)\, \mathrm{e}^{-a_{wi} \left(\frac{\theta_{rad} - SA_{rad}}{\theta_{bd}(\omega_{eng})} \right)^{m_{wi}+1}}}{\theta_{rad} - SA_{rad}} & SA_{rad} < \theta_{rad} \end{cases} \qquad \textbf{(41)}$$

When combustion is considered in addition to the piston work, the dynamics of the internal energy of the gas is described as follows instead of Eq.**(37)**.

$$\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} e_{cyl}(\theta_{rad}) = -p_{cyl}(\theta_{rad}) \left(\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} V_{cyl}(\theta_{rad}) \right) + Q_{\max} \left(\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} x_{burn}(\theta_{rad}) \right) \quad \textbf{(42)}$$

Note that this ordinary differential equation now contains a conditional branch in the second term on the R.H.S.

Combustion with Thermal Exchange between Gas and Wall

Because the temperature of the cylinder wall is kept much lower (at about 80 degrees C) than burning gases (over 2000 degrees C at peak), there is significant amount of thermal energy exchange ΔQ_w between the gas and the cylinder wall, which needs to be added to the combustion dynamics as follows.

$$\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} e_{cyl}(\theta_{rad}) = -p_{cyl}(\theta_{rad}) \left(\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} V_{cyl}(\theta_{rad}) \right) + Q_{\max} \left(\frac{\mathrm{d}}{\mathrm{d}\theta_{rad}} x_{burn}(\theta_{rad}) \right) - \Delta Q_w(\theta_{rad}) \quad \textbf{(43)}$$

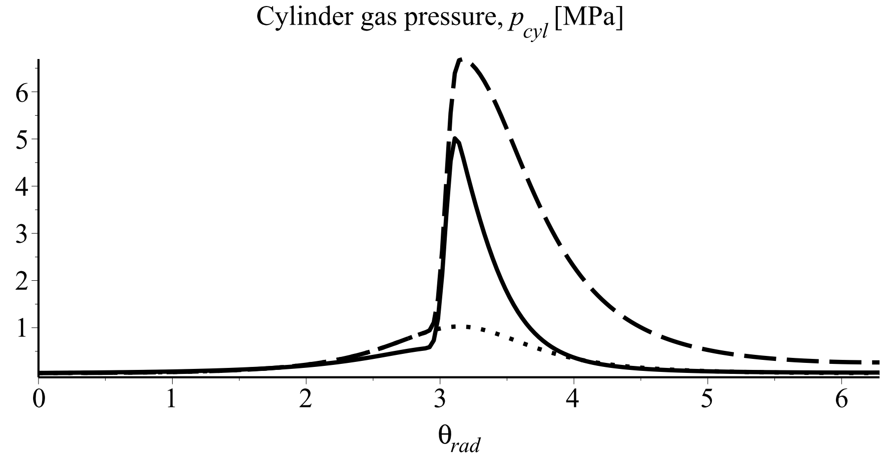
In this paper, a simplistic model is used for thermal exchange just as an example.

$$\Delta Q_w(\theta_{rad}) = k_{therm} \left(T_{cyl}(\theta_{rad}) - T_{wall} \right) \quad \textbf{(44)}$$

where k_{wall} is the thermal conductivity and T_{wall} is the cylinder wall temperature being assumed constant.

Numerical Integration

Now the simulation results of Eqs.**(37)**, **(42)** and **(43)** are shown.



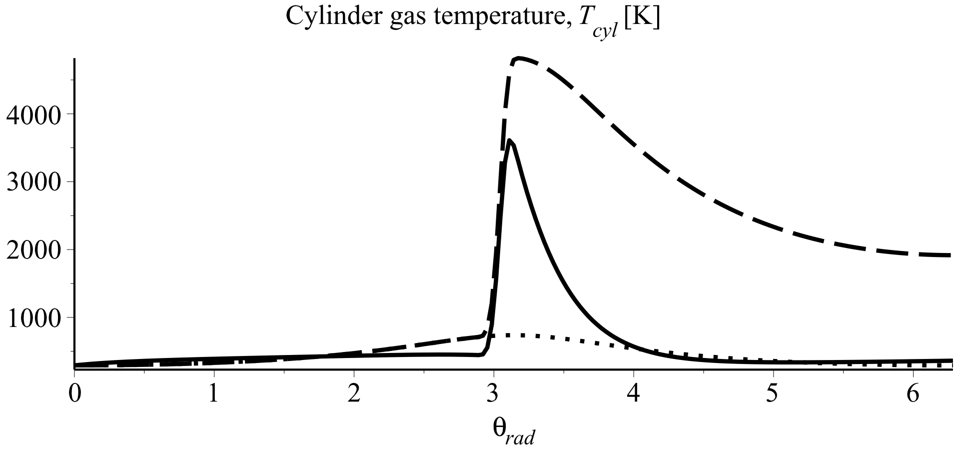


Figure 1. Plots of cylinder gas pressure (top) and temperature (bottom) for an engine cycle, obtained by numerical integration of an ODE for three different cases.

In the above plots for gas pressure and temperature, dotted lines represent adiabatic motoring Eq.**(37)**, dashed lines represent adiabatic combustion Eq.**(42)**, and solid lines represent combustion with thermal exchange Eq.**(43)**.

In the previous section where the combustion chemistry was examined, the pressure and the temperature of the gas were given as operating conditions. Calculations performed in this section may be used to set such operating conditions for chemical equilibrium calculation, thereby enabling the estimation of exhaust emissions from a combustion in engine cycle. However, the challenges listed in the previous section are only partially solved with such an approach. Thus, what has been presented here should be considered as just one baby step forward. Yet, the author would like to emphasize the usefulness of the combined use of symbolic and numeric approaches which greatly speed up comprehension of the problem.

Conclusions

In this paper, the importance and the effectiveness of the integrated use of symbolic and numeric approaches are presented. From the standpoint of the modelling process for the control system development, however, there still remain many other technical aspects that were unfortunately not discussed in this paper.

For example, modelling of chemical reactions occurring in aftertreatment system is as important as that of the combustion chemistry since the combustion and the aftertreatment system are controlled in an integrated manner in the modern engine control system. As for the modelling technologies, modelling a single phenomenon such as a chemical reaction is not even a start of system modelling. As mentioned in the introduction, there are a couple of system modelling technologies that are widely used in automotive industry today [3], [4], [5]. These system modelling technologies have distinctive features such as 1) their own declarative languages to directly describe differential-algebraic equations (DAEs), 2) automatic equation generation mechanism for component connections, known as "acausal" connection, 3) DAE solvers with index-reduction mechanism and support for hybrid-and-stiff system and so on.

Working with these plant modelling technologies is essential when it comes to the development of plant models to meet today's requirements imposed on the control system development, but these technologies are still too much oriented to the numeric approach, and the author believes that the symbolic manipulation technology can be further integrated to the plant modelling as presented in this article so that requirements for plant models can be fulfilled in a more timely manner.

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