Engineering Optimization IV

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Preface


EngOpt2014 is the fourth edition of the biennial scientific meeting “International Conference on Engineering Optimization”. The first conference took place in 2008 in Rio de Janeiro, the second in Lisbon in 2010 and the third in Rio de Janeiro in 2012.

Modern engineering processes and tasks are highly complex, multi and interdisciplinary, requiring the cooperative effort of different specialists from engineering, mathematics, computer science and even social sciences. Optimization methodologies are fundamental instruments to tackle this complexity, giving us the possibility to unite synergistically team members’ inputs and thus decisively contribute to solve the new engineering technological challenges. With this context in mind, the main goal of this EngOpt conference is to join engineers, applied mathematicians, computer and other applied scientists working on research, development and practical application of optimization methods applied to all engineering disciplines, in a common scientific forum to present, analyze and discuss their latest developments.

The contributing papers are organized around the following major themes:

- Numerical Optimization Techniques
- Design Optimization and Inverse Problems
- Efficient Analysis and Reanalysis Techniques
- Sensitivity Analysis
- Industrial Applications

And the mini-symposiums:

- MS01 – Topology Optimization For Structural Static and Dynamic Failures (Organized by Gil Ho Yoon, Matteo Bruggi and Emílio Carlos Nelli Silva)
- MS02 – Optimization in Oil and Gas Industries (Organized by Silvana Bastos and Bernardo Horowitz)
- MS03 – New Advances in Derivative-Free Optimization Methods for Engineering Optimization (Organized by J.F.A. Madeira and A.L. Custódio)
- MS04 – Optimization Methods in Biomechanics and Biomedical Engineering (Organized by P.R. Fernandes and J. Folgado)
- MS05 – Optimization of Laminated Composite Materials (Organized by H.C. Rodrigues and A.L. Araújo)
- MS06 – Inverse Problems in Engineering (Organized by Schalk Kok and Daniel N. Wilke)

We want to take this opportunity to extend our recognition to the mini-symposium organizers, scientific committee members, session chairs, lecturers and conference participants for the scientific success of this event, the many interesting presentations and active participation in the discussions that were the main objectives of this scientific meeting.

Our indebtedness is also due to Ms. Andrea de Freitas and Ms. Anabela Arenga for all their efforts and commitment to the successful running of the conference.

The Editors,
Lisbon, Instituto Superior Técnico, September 2014
Organizers

Bayesian estimate of mass fraction of burned fuel in internal combustion engines using pressure measurements

Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

R.N. Carvalho
Petrobras Research Center, Rio de Janeiro, Brazil

G.S. Dulikravich
Florida International University, Miami, USA

ABSTRACT: The numerical simulation of combustion processes in internal combustion engines is a very difficult task. It involves the reacting turbulent flow of a gaseous mixture that compresses and burns in a short amount of time. Different models, with various levels of complexity, exist in the open literature and usually need calibration to work properly. Although being quite simple, a First Law analysis of this problem is widely used by the industry. Such formulation requires a model for the mass fraction of burned fuel, which is often based on the Wiebe equation, and requires calibration using experimental data. The objective of this paper is to estimate the mass fraction of burned fuel using Bayesian particle filters. Particle filters, also called Sequential Monte Carlo (SMC) methods, fit into the domain of inverse modelling procedures, where measurements are incorporated into a computational model so as to formulate some feedback information on the uncertain model state variables and/or parameters, through accurate representations of their probability density functions. Based on a simple sampling importance distribution and resampling techniques, particle filters combine Monte Carlo samplings with sequential Bayesian filtering problems. In this particular application, measurements obtained from a pressure transducer located inside a combustion chamber are used to feed an observation model, while a First Law analysis is used as an evolution model to this Bayesian estimate. Very good results are obtained for the mass fraction of burned fuel, showing the great potential for this technique to be used as practical tool in the industry.

1 INTRODUCTION

Internal combustion engines play a vital role in modern society. Although the use of alternative energy sources (wind, solar, etc.) has increased in recent years, fossil fuels are still being massively used, mainly due to their high energy content per unit volume. Thus, the optimization of actual engines is of utmost importance to maximize their performance and also decrease the gaseous and particulate matter emissions to the environment.

The complete numerical simulation of combustion in internal combustion engines is a very complex task, involving a turbulent and unsteady flow of a reacting non-homogeneous mixture with temperature dependent physical properties. Thus, there are some classes of models described on the literature, depending on the level of simplifications adopted (Fergunson 1986, Heywood 1988).

Although being very simple, one of the combustion models widely used by the industry and academia consider the burned and non-burned gases as being a homogeneous ideal gas, with uniform temperature and pressure. This model, derived from the First Law of Thermodynamics, is known as zero-dimensional model (Fergunson 1986, Heywood, 1988). In order to predict the rate of energy released by the fuel, such model usually employs some empirical or semi-empirical equation to model the mass fraction of burned fuel, being the Wiebe’s equation the most commonly used (Murayama et al. 1982, Miyamoto et al. 1985, Fergunson 1986, Heywood 1988). Also, to take into account the energy lost by the combustion chamber walls, usually an empirical time dependent heat transfer coefficient is used (Fergunson 1986, Borman & Nishiwaki 1987, Heywood 1988).

The main problem with this formulation is the need to adjust some parameters in the Wiebe’s equation, in order to make the numerical pressure curve match the experimental one. Also, as reported by Borman and Nishiwaki (1987), correlations for the heat transfer coefficient that were obtained for a specific engine running under specific conditions, in general do not apply for other engines and present discrepancies over 100% among them.
Finally, it is worth mentioning that, recently, other works also proposed some procedures to estimate the mass fraction of burned fuel (Mendera et al. 2002, Mittal et al. 2008, Yeliana et al. 2008b, Yeliana et al. 2008a, Mittal et al. 2009, Yeliana et al. 2011, Catania et al. 2011, Dogah 2012, Chung et al. 2013, Finesso & Spessa 2014), but none of them used Bayesian techniques.

2 PHYSICAL PROBLEM

The physical problem considered here involves the combustion process in a spark ignition internal combustion engine. Initially the combustion chamber is filled with a pre-mixed mixture of fuel and air at a stoichiometric ratio with both the inlet and exhaust valves closed. The piston then moves upwards, from the bottom dead center (BDC) to the top dead center (TDC). The linear position of the piston is converted into an angular movement as shown in Figure 1, such that the crankshaft angle \( \theta \) is equal to 0° when the piston is located at the TDC and ±180° when it is at the BDC.

The mixture of fuel and air is ignited by a spark at a pre-defined angle \( \theta_i \), and the combustion continues for a period \( \Delta \theta \). The angle \( \theta \), in radians, is related to time \( t \), in seconds, through the following relationship:

\[
\theta = \frac{t}{2\pi N}
\]

where \( N \) is the angular velocity of the crankshaft, in Hertz. Once the combustion is started, there is a heat release from the fuel to the combustion chamber volume, which makes the pressure and temperature rises. Such heat is transformed into work through the movement of the piston downwards, which is transferred to the crankshaft. Since the combustion chamber walls and the piston head must be cooled, heat is also transferred, mainly by convection, to these regions.

The objective of this work is to estimate the temporal heat release rate of fuel, using pressure measurements taken inside the combustion chamber.

In order to numerically simulate the combustion process of this engine, a zero-dimensional model, based on the First Law of Thermodynamics, was used for the processes occurring inside the combustion chamber. The gas inside the cylinder was considered an ideal gas with uniform properties. From the equation of state for an ideal gas, together with the First Law of Thermodynamics, the following equation can be obtained, when both the inlet and outlet valves are closed:

\[
\frac{dP}{d\theta} = \frac{\gamma}{V} \frac{dV}{d\theta} + \frac{(\gamma - 1)}{V} \frac{dQ}{d\theta}
\]

where \( P(\theta) \) is the time-varying pressure, \( \theta \) is the crankshaft angle (which is related to time), \( V(\theta) \) is the instantaneous volume of the cylinder (which can be obtained from the engine speed and geometrical data), \( Q(\theta) \) is the heat released and \( \gamma \) is the polytropic coefficient, which was assumed constant and equals to 1.33 in this work.

For the calculation of the pressure inside the cylinder as a function of the crankshaft angle, it is necessary to obtain the value of the heat release rate, appearing in Eq. (2). One of the most used expressions encountered in the literature uses the Wiebe’s function model (Fergunson 1986, Heywood 1988), given by

\[
\frac{dQ}{d\theta} = Q_{\text{total}} \frac{dx}{d\theta} - \frac{dQ_w}{d\theta}
\]

\[
x(\theta) = 1 - e^{-\left(\frac{\theta - \theta_i}{\Delta \theta}\right)^n}
\]

where \( x \) is the mass fraction of burned fuel. The parameter \( a \) controls the combustion duration, \( m \) controls the combustion evolution, \( \theta_i \) is the crankshaft angle where the combustion starts, \( \Delta \theta \) is the combustion duration, and \( Q_{\text{total}} \) is the total amount of heat released, given by the mass of injected fuel times its lower heating value (considering a combustion with 100% of efficiency). Parameters \( a \) and \( m \) usually have to be obtained by trial and error, by some optimization method (Colaço et al. 2010a, Colaço et al. 2010b), or even be estimated together with the heat transfer coefficient through the combustion chamber walls.

The wall heat loss can be modeled through an overall time dependent heat transfer coefficient \( h(\theta) \)

\[
Q_w = hA(T - T_{\text{gas}})
\]

where \( T(\theta) \) is the wall temperature, \( T_{\text{gas}} \) is averaged gas temperature, and \( A(\theta) \) is the combustion chamber surface area. Several correlations for such heat transfer coefficient at the gas-walls surfaces are available in the literature (Fergunson 1986, Borman and Nishiwaki 1987, Heywood 1988). It is worth mentioning that the estimate of the heat transfer coefficient is a complex problem itself and was already discussed by authors in (Hamilton et al. 2014).

In this paper, we used synthetic data for the measured pressure, obtained through the solution of Eq. (2) with a known transient variation of the heat transfer coefficient profile and also with “known” values of...
\( a = 1.2 \) and \( m = 0.8 \) in the Wiebe’s equation. In order to generate such data, the Woschni’s model (Ferguson 1986, Borman & Nishiwaki 1987, Heywood 1988), given as

\[
h(W/m^2K) = 3.26B(m^{-0.2})P(kPa)^{0.5}T(K)^{-0.55}w(m/s)^{0.8} \tag{5}
\]

was used, where \( B \) is the bore of the cylinder and \( w \) is the average cylinder gas velocity, which, for a four-stroke, water-cooled engine, can be expressed as (Heywood 1988, Ferguson 1986, Borman and Nishiwaki 1987)

\[
w = \left[ C_1S_p + C_2 \frac{V_d T_r}{P V_r} (P - P_m) \right] \tag{6}
\]

where \( V_d \) is the displaced volume, \( P_r \), \( V_r \) and \( T_r \) are taken at some reference state, \( P_m \) is the motored cylinder pressure at the same crank angle as \( P \), and the constants \( C_1 \) and \( C_2 \) are given as:

- Gas exchange: \( C_1 = 6.18; C_2 = 0 \)
- Compression: \( C_1 = 2.28; C_2 = 0 \)
- Combustion and expansion: \( C_1 = 2.28; C_2 = 3.24 \times 10^{-3} \)

After the models of the heat release rate given by Eq. (3) and the wall heat losses given by Eqs. (4)–(7) have been defined, the pressure versus crankshaft angle curve for a closed cycle can be obtained through the solution of Eq. (2), by using some integration technique, such as a fourth order Runge-Kutta scheme, which was implemented in this work, for an engine whose parameters are given in Table 1. The numerically generated pressure curve was validated against experimental data (Hamilton et al. 2014) with very good agreement between the results.

In our previous work (Hamilton et al. 2014), we estimated the heat transfer coefficient through the walls of the combustion chamber, with excellent results. We also demonstrated that the sensitivity of pressure related to the heat transfer coefficient is very low.

### Table 1. Engine parameters (Melo et al. 2007).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine manufacturer</td>
<td>Volkswagen</td>
</tr>
<tr>
<td>Engine model</td>
<td>1.8 AP, Flex</td>
</tr>
<tr>
<td>Fuel</td>
<td>Gasoline</td>
</tr>
<tr>
<td>Number of cylinders</td>
<td>4</td>
</tr>
<tr>
<td>Valves per cylinder</td>
<td>2</td>
</tr>
<tr>
<td>Bore</td>
<td>81.01 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>86.4 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>144 mm</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>11</td>
</tr>
<tr>
<td>Speed</td>
<td>2500 rpm</td>
</tr>
<tr>
<td>Torque</td>
<td>75 N.m (gasoline)</td>
</tr>
<tr>
<td>Imep</td>
<td>5.22 bar</td>
</tr>
<tr>
<td>Rated power</td>
<td>76 kW (gasoline)</td>
</tr>
<tr>
<td>Inlet closing valve</td>
<td>164° BTDC</td>
</tr>
<tr>
<td>Outlet opening valve</td>
<td>146° ATDC</td>
</tr>
</tbody>
</table>

In other words, large variations of \( h(\theta) \) cause very small variations in the pressure curve. Nevertheless, the results previously presented in were very good even considering such low sensitivity. In this work, on the other hand, we consider a known variation of \( h(\theta) \) and the objective is thus to estimate the time variation of mass fraction of burned fuel \( x(\theta) \).

### 3 INVERSE PROBLEM

The inverse problem considered in this work is formulated in the Bayesian framework, where the results are obtained in terms of the posterior probability density, which is the conditional probability of the unknown variables \( y \) given the measurements \( z \).

If the measurement errors follow a Gaussian distribution with zero mean, covariance matrix \( W_e \), and are additive and independent of the unknown variables \( y \), the model for the measurements, which gives the probability of the measurements \( z \) given the unknown variables \( y \), is obtained by the likelihood function (Kaipio & Somersalo 2004, Maybeck 1979)

\[
\pi(z|y) = (2\pi)^{-n/2}|W_e|^{-1/2}\exp\left[-\frac{1}{2}(z-f(y))^T W_e^{-1} (z-f(y))\right] \tag{8}
\]

where \( f(y) \) is the solution of the direct (forward) problem. Such solution is obtained from the mathematical formulation of the problem under analysis with known \( y \).

The posterior probability density is related to the prior model, which is the model for the unknowns without the information obtained by the measurements, and the likelihood function by means of the Bayes’ theorem (Maybeck 1979, Kaipio & Somersalo 2004)

\[
\pi_{\text{posterior}}(y) = \pi(y|z) = \frac{\pi(y)f(z|y)}{\pi(z)} \tag{9}
\]

where \( \pi_{\text{posterior}}(y) \) is the posterior probability density, \( \pi(y) \) is the prior density, \( \pi(z|y) \) is the likelihood function and \( \pi(z) \) is the marginal probability density of the measurements, which plays the role of a normalizing constant.

The Bayes’ theorem is the base for the state estimation problem, also referred as non-stationary inverse problems (Maybeck 1979). These problems use the available measurement data, and the prior information about the physical phenomena and the measurement device, to produce estimates of the dynamic variables, sequentially.

State evolution problems are based on two models: the evolution model and the observation model. The first one is related to the prior information about the data, while the second is associated to the model for the measurements.

The evolution model for the state variables \( y \) can be written as

\[
y_{e} = f_{e}\left(y_{e-1}, y_{k}\right) \tag{10}
\]
The objective of this work is to estimate the transient heat release rate inside the combustion chamber of a spark ignition internal combustion engine using pressure measurements. In the context of the state estimation, the state variables are then the pressure inside the combustion chamber, and the heat release rate of the fuel, given as:

\[
\dot{Q}_{\text{fuel}} = -\frac{dQ_{\text{fuel}}}{dt} = Q_{\text{total}} \frac{dx}{d\theta}
\]  

where \( f \) is, in the general case, a non-linear function of \( y \) and of the state noise or uncertainty vector given by \( v_k \in \mathbb{R}^n \). The vector \( y_k \in \mathbb{R}^n \) is called the state vector and contains the variables to be dynamically estimated. This vector advances in time in accordance with the state evolution model (10). The subscript \( k = 1, 2, 3, \ldots \) denotes a time instant \( t_k \) in a dynamic problem.

The second model, named observation model, represents the relation between the state variables \( y \) and the measurements \( z \), by means of a general function \( h \):

\[
z_k = h(y_k, \pi) \tag{11}
\]

where \( z_k \in \mathbb{R}^{nz} \) are available at times \( t_k, k = 1, 2, 3, \ldots \). Eq. (11) is referred to as the observation/measurement model. The vector \( \pi_k \in \mathbb{R}^{nz} \) represents the measurement noise or uncertainty.

The combination of the evolution and observation models, through the Bayes’ theorem, generate a dynamic estimate of the state variables \( x \) in time, by means of a sequence of calculations involving two steps: a prediction, using the prior probability density, and an update, using the likelihood function in conjunction with the Bayes’ theorem. This procedure is known as filtering problem (Maybeck 1979, Kaipio & Somersalo 2004).


The main idea in the particle filter is to represent the required posterior density function by a set of random samples with associated weights and to compute the estimates based on these samples and weights (Ristic et al. 2004). In this paper we used the SIR algorithm, whose steps are briefly shown in Table 2. More details of this algorithm can be found in (Ristic et al. 2004).

**Table 2.** SIR Algorithm (Ristic et al. 2004).

**Step 1**

For \( i = 1, \ldots, N \) draw new particles \( y_i^k \) from the prior density \( \pi(y_1^k | y_{k-1}^k) \) and then use the likelihood density to calculate the correspondent weights \( w_i^k = \pi(z_k | y_i^k) \).

**Step 2**

Calculate the total weight \( i = \sum_i w_i^k \) and then normalize the particle weights, that is, for \( i = 1, \ldots, N \) let \( w_i^k = r^{-1} w_i^k \).

**Step 3**

Resample the particles as follows:

1. Construct the cumulative sum of weights (CSW) by computing \( c_i = c_{i-1} + w_i^k \) for \( i = 1, \ldots, N \), with \( c_0 = 0 \).
2. Let \( i = 1 \) and draw a starting point \( u_i \) from the uniform distribution \( U[0, N^{-1}] \).
3. For \( j = 1, \ldots, N \) move along the CSW by making \( u_j = u_i + N^{-1}(j-1) \).
4. While \( u_j > c_i \), make \( i = i + 1 \).
5. Assign sample \( x_i = x_i^k \).
6. Assign sample \( w_i^k = N^{-1} \).

Thus, for the state vector \( y \) we have:

\[
y = \{ P, \dot{Q}_{\text{fuel}} \} \tag{13}
\]

The state evolution for the pressure \( P(\theta) \) is given by the solution of Eqs. (2–7), given \( x(\theta) \) and \( h(\theta) \). In this paper we considered a Wegchini’s correlation for \( h \) (Ferguson 1986, Borman & Nishiwaki 1987, Heywood 1988), whereas for the heat release rate we do not have an explicit state evolution model. Also, in order to make the estimate very general, we did not use the Wiebe’s equation for \( x(\theta) \) (Ferguson 1986, Heywood 1988), but considered an artificial state evolution model, given as a random walk model for the heat release rate:

\[
\dot{Q}_{\text{fuel}}(\theta_k) = \dot{Q}_{\text{fuel}}(\theta_{k-1}) + \sigma_g \varepsilon \dot{Q}_{\text{fuel}}(\theta_{k-1}) + \sigma_o \varepsilon \tag{14}
\]

where \( \sigma_g \) is the step size of the random walk (taken as 0.1), \( \varepsilon \) is random variable with zero mean and uniform distribution between −1 and 1, and \( \sigma_o \) is a bias (taken as 1), added to the model to avoid the convergence to zero at initial times (where there is no release of rate). The initial guess is given as a Gaussian distribution with zero mean and zero variance.

For the observation model, we considered synthetic measured pressures, obtained with a known variation of \( x(\theta) \). Also, in order to take into account the presence of noise, we added a Gaussian fluctuation in the pressure given by

\[
P_{\text{meas}}(\theta) = P_{\text{calc}}(\theta) + \sigma_{\text{meas}} \varepsilon \tag{15}
\]

where \( P_{\text{calc}}(\theta) \) is the exact value of the pressure obtained by the solution of Eq. (2) with the exact value.
Table 3. Test-cases analyzed.

<table>
<thead>
<tr>
<th>Test-case</th>
<th>$\sigma_{\text{meas}}$ (bar)</th>
<th>Measurement frequency (Hz)</th>
<th>Number of particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>$1 \times 10^5$</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>200</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td>400</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td>800</td>
</tr>
<tr>
<td>5</td>
<td>$5 \times 10^4$</td>
<td></td>
<td>100</td>
</tr>
<tr>
<td>6</td>
<td>0.2</td>
<td>$5 \times 10^4$</td>
<td>100</td>
</tr>
</tbody>
</table>

Figure 2. Mean of the RMS error for test cases 1 through 4.

of $x(\theta)$, $\sigma_{\text{meas}}$ is the standard deviation of the simulated measurements, and $\xi$ is a random variable with Gaussian distribution and zero mean.

In this paper we analyzed different number of particles and measurement frequencies. Table 2 summarizes such cases.

Since the particle filter estimate relies on several random numbers, we used the procedure presented in (Hamilton et al., 2014) to check its convergence, where the estimation was performed 100 times for each test case and an averaged RMS error and CPU time were obtained, where the RMS error for each run was defined as

$$RMS = \sqrt{\frac{1}{K} \sum_{k=1}^{K} \left[ \dot{Q}(\theta_k) - \dot{Q}_{\text{sim}}(\theta_k) \right]^2}$$  \hspace{1cm} (16)

where $K$ is the final time used for comparison between the estimated and exact value of the heat release rate of the fuel.

Figure 2 presents the average value of the RMS error for the test cases 1 through 4 presented in Table 1. As expected, as the number of particles increase, the error of the solution decrease. It is worth mentioning that the reduction of the error is more intense when the number of particles increases from 100 to 200 and then to 400. The reduction from 400 to 800 particles is less pronounceable.

The mean value of the CPU time for test cases 1 through 4, considering 100 repetitions for each test case, is presented in Figure 3. The code was written in Matlab and ran on a i7 3.4 GHz with 8Gb of RAM memory. The time required for the solution range from a few seconds to a case with 100 particles to almost half hour to 800 particles.

Figure 4 shows the results for test case 1 (100 particles) and Figure 5 for test case 4 (800 particles), where a frequency of measurements equal to 100 kHz was used, considering a standard deviation of 0.1 bar in the measurements. As once can see, there is no visual difference between these results. Such conclusion could also be made from the analysis of Figure 2, where the reduction of RMS from 100 to 800 particles is less than 5%. It is remarkable then that with only 100 particles, which took just a few seconds to run, the estimate of heat release rate is very good, especially at the start of the combustion, where the filter captures very well the very fast release of heat.

One interesting practical aspect to be analyzed is the influence of the measurement frequency on the final results. Figure 6 shows the results for test case 5, where 100 particles where used for a frequency of measurements equal to 50 kHz. Even in this case where
half of the original measurement frequency was used, the heat release rate is very well captured.

Finally, a last test case was analyzed (test case 6) where we increased the level of noise from 0.1 bar to 0.2 bar. For this test case we used 100 particles with a frequency of measurements equal to 50 kHz. Figure 7 shows the results for this test case where the estimate is very good, although the confidence intervals are wider than the ones presented in test case 5. Figure 8 shows the estimated pressure curve, where one can see that it is also very well capture by the present technique.

5 CONCLUSIONS

In this paper we applied a Bayesian particle filter to estimate the heat release rate of fuel in a spark ignition internal combustion engine. Pressure data were used as measurements, which contained different levels of errors and were available at different measurement frequencies. Results show that the method is capable to recover the unknown function with a few particles, even in the regions where the release of heat is very fast. Considering that many industrial applications rely on empirical or semi-empirical expressions for the heat release rate, the methodology presented in this paper might have a great impact on those applications, since it is automatic and do not rely on any interference from the user.

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