EFFECT OF THE REYNOLDS AND LEWIS NUMBER TO THE FUEL DROPLET VAPORIZATION

by

Habib MEROUANE*

Department of Mechanical Engineering, Faculty of Science and Technology University of Mascara, Mascara, Algeria

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In this work we present the effect of Reynolds and Lewis numbers on the fuel droplet vaporization of n-heptane. This study allows us to fully understand the vaporization phenomenon of fine fuel droplets (spray) in energy systems in order to improve combustion efficiency, reduce the formation of pollutants and unburned materials such as CO and NO_x . The study is based on an analytical solution of the governing equations of the vaporization process by calculating the droplet diameter evolution, the temperature at the surface of the droplet, the mass fraction of fuel vapor and the mass-flow rate. The analytical results obtained by the theoretical model are compared to the experimental data in order to validate our results.

Key words: droplet vaporization, droplet, fuel droplets, droplet combustion

Introduction

The study of the vaporization and combustion processes of liquid fuel droplets plays a very important role in energy systems such as industrial furnaces, gas turbines, Diesel engines, and liquid-propelled rocket engines. In these systems the vaporization process is dominant, the fuel is injected into the combustion chamber as a spray using the injector. The spray is made up of fine liquid fuel droplets of different sizes. The fuel vapors mix with the gaseous oxidizer to form the reactive mixture which ignites to produce the spray combustion. Although the large droplets have the possibility to burn individually, then it is probable that it is the phenomenon of the droplet's vaporization which imposes the time and length scales of the combustion chambers [1]. To better understand and apprehend the vaporization process, it is necessary to study a single droplet of a liquid fuel in the simple case, the vaporization of a single immobile droplet, introduced into a hot surrounding environment. The temperature and the pressure at the surface of the liquid fuel droplet are lower than the surrounding environment. There will appear a heat transfer by conduction and diffusion between the ambient environment and the surface of the droplet. A part of this energy is transferred inside the droplet and serves to heat it. The other part is used to vaporize the liquid on the surface of the droplet such that a zone of vapor concentration is created around the droplet, the fuel vapor concentration gradient between the surface of the droplet and the gas environment is large and the vapor diffuses into the gas environment, and the process of vaporization continues.

^{*}Author's e-mail: mer_habib@yahoo.fr

The vaporization of a fuel droplet is usually treated by using a quasi-steady theory [2, 3]. This hypothesis is based that the flow and the transfer of mass and energy adapt immediately at each instant to the local boundary conditions.

Much progress has been made to understanding the vaporization of liquid fuel droplet over the past years since the work of Sirignano [4], Aggarwal *et al.* [5], Hiroshi *et al.* [6], Li and Zhang [7], Chiang *et al.* [8], *Shuen et al.* [9], and recently the work of Cameron and Birouk [10], Fang *et al.* [11], Muelas *et al.* [12], Patel and Sahu [13], Zihe *et al.* [14], Yu and Chen [15], Wang *et al.* [16], and Luo *et al.* [17].

Chauveau *et al.* [18] studied the validity of the d^2 law of the droplet vaporization in normal and microgravity condition and stagnant hot atmospheric environment, the temperature varied in the range up to 967 K. They observed that the d^2 law is fails in microgravity environment at ambient temperatures below 950 K and they observed also that the droplet duration is longer in microgravity than in normal gravity under the same ambient test conditions. The experimental results make evident that for temperatures exceeding around 950 K, the d^2 law holds throughout the entire droplet duration, and the mass transfer rate is identical in both microgravity and normal gravity environment.

Birouk and Toews [19] studied the effect of the initial diameter on the vaporization rate of a fuel droplet in a turbulent atmosphere. Their experimental results showed that, at ambient pressure and temperature, there is no effect on the droplet vaporization process by the suspension fiber technique, but the initial diameter of the droplets exerts an apparent effect on the vaporization rate of the droplets. They also observed that after using the statistical data, a correlation in terms of Damkohler number was found between the droplet vaporization rate, the droplet size and the intensity of the turbulence. Surprisingly, the expression of this correlation is similar for heptane and decane.

Chauveau *et al.* [20] studied the effect of the droplet carrier fiber on the droplet evaporation process. This effect is evaluated for a droplet evaporating in a hot environment at atmospheric pressure using the test conditions and experimental configurations with variation in the diameter of the droplet support fiber which varies between 14 μ m and 225 μ m. The ambient temperature explored in these studies ranges from ambient temperature up to 973 K. The *n*-heptane is chosen because it is the most commonly used fuel. The main results are that the cross-fiber technique, which uses fiber diameters of 14 μ m, does not induce any noticeable heat transfer in the droplet and, therefore, does not interfere with the evaporation process. In contrast, the conventional fiber technique, which uses relatively coarser fibers, greatly improves the rate of droplet evaporation due to increased conduction heat transfer through the fiber. A correlation is proposed to quantify the level of this increase as a function of ambient temperature and fiber cross-section.

Pinheiro *et al.* [21] studied the effects of ambient temperature, pressure and fuel vapor concentration of the ethanol droplet. Their results indicate that the increasing of the ambient pressure causes an increase in the ratio of the initial heating time to the total evaporation lifetime, which enhances the unstable effects of droplet evaporation. The results also show that under ambient temperatures above 600 K, the evaporation rate increases with increasing ambient pressure, contrary to what happens for cases where the ambient temperature is below 600 K.

The motivation of the present work is to make the effect of the Lewis and Reynolds numbers to the droplet vaporization by calculating the mass-flow and the variation of the droplet diameter for the stagnant case at high temperature, then for the stagnant case for different Lewis number and in the convection case for different Reynolds number. The estimation of the

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thermodynamic properties of the gas phase around the droplet during its vaporization is calculated at the reference temperature by the 1/3 rule. The study is based on an analytical solution by resolving the governing equations that controls the phenomenon and the process of vaporization. In this study, an algorithm with FORTRAN program is adopted to determine the variation of the droplet diameter, surface temperature, mass fraction of fuel vapor and the mass-flow rate. The results obtained by the analytical theory are tested with experimental data for the variation of the droplet diameter obtained by Hiroshi *et al.* [6].

Mathematical model and hypothesis

We suppose in this study a unique fuel volatile droplet, introduced into a stationary environment of hot and ambient air with constant and uniform pressure. The droplet is spherical with a uniform temperature; the gas liquid interface is at phase equilibrium. The droplet is heated by conduction and convection. The mathematical formulation for the droplet vaporization process is composed of the mass and energy conservation for the two-phase liquid droplet and the gaseous mixture of fuel vapor and air, fig. 1.



Figure 1. Droplet vaporization process

Mass conservation equation

The mass conservation equation for fuel vapor is given:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho_{\rm g}r^2u\right) = 0\tag{1}$$

where *u* is the relative velocity to the droplet surface, *r* – the droplet radius, and ρ_g – the density of the ambient environment:

$$4\pi r^2 \rho_{\rm g} u = \dot{m} \tag{2}$$

where \dot{m} is the mass-flow rate of vaporization.

Mass species equation

During the process of vaporization, the species composing the liquid is transported through the liquid-gas interface by a change of state, from the liquid state to the vapor state. The continuity of the mass flux for the species of the droplet is given [22]:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho_{\rm g}uY_{\rm F}\right) - \frac{1}{r^2}\frac{\partial}{\partial r}\left(\rho_{\rm g}r^2D_{\rm m}\frac{\partial Y_{\rm F}}{\partial r}\right) = 0 \tag{3}$$

where Y_F is the mass fraction of fuel vapor and D_m – the molecular diffusion coefficient of the vapor in the ambient environment. The balance at the surface of the droplet shows that the evaporated flow \dot{m} is composed of a convection term:

$$4\pi r_{\rm s}^2 \rho_{\rm g} u Y_{\rm F}^{\rm s} \tag{4}$$

and a diffusion term:

$$-4\pi r_{\rm s}^2 \rho_{\rm g} D_{\rm m} \frac{\partial Y_{\rm F}}{\partial r}\Big|_{r=r_{\rm s}}$$
⁽⁵⁾

and

$$\dot{m} = 4\pi r_{\rm s}^2 \rho_{\rm g} u Y_{\rm F}^{\rm s} - 4\pi r_{\rm s}^2 \rho_{\rm g} D_{\rm m} \left. \frac{\partial Y_{\rm F}}{\partial r} \right|_{r=r_{\rm s}} \tag{6}$$

where $Y_{\rm F}^{\rm s}$ is the fuel mass fraction at the droplet surface.

The integration of the eq. (3) with the following boundary conditions gives the expression of the mass fraction and the mass-flow rate of vaporization [23]:

$$r = r_{\rm s}, \ T = T^{s}, \ Y_{\rm F} = Y_{\rm F}^{\rm s}$$

$$r = \infty, \ T = T^{\infty}, \ Y_{\rm F} = Y_{\rm F}^{\infty}$$

$$Y_{\rm F} = 1 - \exp\left(-\frac{\dot{m}}{4\pi\rho_{\rm g}D_{\rm m}r}\right)$$
(7)

where $Y_{\rm F}$ is the fuel mass fraction:

$$\dot{m} = 4\pi r \rho_{\rm g} D_{\rm m} \ln\left(1 + B_{\rm M}\right) \tag{8}$$

where B_M is the mass transfer number or the Spalding number [2] defined:

$$B_M = \frac{Y_{\rm F}^{\rm s} - Y_{\rm F}^{\infty}}{1 - Y_{\rm F}^{\rm s}} \tag{9}$$

We can introduce the Lewis number in eq. (8) and the mass-flow rate can be written:

$$\dot{m} = 4\pi r \frac{\lambda_{\rm g}}{{\rm Le}C_{p_{\rm g}}} \ln(1 + B_M) \tag{10}$$

Where Le is the Lewis number defined:

$$Le = \frac{\lambda_g}{D_m \rho_g C_{\rho_g}}$$
(11)

The expression of the variation of the droplet squared diameter during its vaporization as function of time in quasisteady is defined [22]:

$$\frac{\mathrm{d}D^2}{\mathrm{d}t} = -8\frac{\rho_{\rm g}}{\rho_L}D_{\rm m}\ln(1+B_M) \tag{12}$$

and

$$K = -8\frac{\rho_{\rm g}}{\rho_L}D_{\rm m}\ln(1+B_M) \tag{13}$$

where *K* is the droplet vaporization rate.

In the presence of the convection, the mass-flow rate of vaporization is given [22]:

$$\dot{m} = 2\pi \rho_{\rm g} D_{\rm m} r_{\rm s} {\rm Sh}_0 \ln(1 + B_M) \tag{14}$$

were Sh₀ is the Sharwood number difined [24]:

$$Sh_0 = 2 + 0.6 \operatorname{Re}_d^{1/2} Sc^{1/3}$$
(15)

With

$$\operatorname{Re}_{d} = \frac{2\rho_{g} \left| U_{g} - U_{d} \right| r_{s}}{\eta}$$
(16)

and

$$Sc = \frac{\eta}{D_{\rm m} \rho_{\rm g}} \tag{17}$$

where Sc is the Schmidt number, Re_{d} – the Reynolds number, U_{g} – the velocity of the ambient environment, U_{d} – the velocity of the droplet, and η – the kinematic viscosity of the ambient environment. The physical properties are calculated at reference temperature.

Energy conservation equation:

The energy conservation equation is given [22]:

$$r^{2}\rho_{g}uC_{p_{g}}\frac{\partial T}{\partial r} = \frac{\partial}{\partial r}\left(r^{2}\lambda_{g}\frac{\partial T}{\partial r}\right)$$
(18)

where C_{p_g} is the specific heat of the vapor and λ_g – the thermal conductivity of the gaseous film, a balance on the surface of the droplet shows that the flow of thermal energy arriving on the droplet Q_g serves on the one hand to heat the droplet Q_l and on the other hand to the process evaporation mL_{vap} :

$$Q_{\rm g} = Q_l + \dot{m}L_{\rm vap} \tag{19}$$

If the heat of the droplet is ignored we can write:

$$4\pi r_{\rm s}^2 \lambda_{\rm g} \left. \frac{\partial T}{\partial r} \right|_{r=r_{\rm s}} = \dot{m} L_{\rm vap} \tag{20}$$

By integration of the eq. (18) and using the relation (20) with the following boundary conditions, we can find the relation of the profiles of temperature and mass-flow rate in quasi-steady [25].

Boundary conditions:

$$r = r_{\rm s}, \ T = T^{\rm s}, \ Y_{\rm F} = Y_{\rm F}^{\rm s}$$

$$r = \infty, \ T = T^{\infty}, \ Y_{\rm F} = Y_{\rm F}^{\infty}$$

$$T = \frac{\left(T^{\rm s} - T^{\infty}\right)}{\exp\left(-\frac{\dot{m}C_{\rm vap}}{4\pi\lambda_{\rm g}r_{\rm s}}\right) - 1} \left[\exp\left(-\frac{\dot{m}C_{\rm vap}}{4\pi\lambda_{\rm g}r}\right) - 1\right] + T_{\infty}$$
(21)

$$\dot{m} = 4\pi r_{\rm s} \rho_{\rm g} D_{\rm m} \ln\left(1 + B_{\rm T}\right) \tag{22}$$



Figure 2. Droplet vaporization algorithm

Mass transfer number

For the boundary conditions:

r

with

$$B_T = \frac{C_{p_{\rm g}} \left(T_{\infty} - T_{\rm s} \right)}{L_{\rm vap}} \tag{23}$$

By taking account the convective effect, the mass-flow rate and heat transfer energy can be writing by the expressions' given [22]:

$$\dot{m} = 2\pi r_{\rm s} \rho_{\rm g} D_{\rm m} \mathrm{Nu}_0 \ln\left(1 + B_T\right) \tag{24}$$

$$Q_{\rm g} = 2\pi\lambda_{\rm g}r_{\rm s}^{\rm s} {\rm Nu}_0 \left(T^{\infty} - T^{\rm s}\right) \frac{\ln\left(1 + B_T\right)}{B_T} \qquad (25)$$

where

$$Nu_0 = 2 + 0.6 \operatorname{Re}_d^{1/2} \operatorname{Pr}^{1/3}$$
(26)

with

$$\Pr = \frac{\eta C_{Pg}}{\lambda_{g}}$$
(27)

where Nu_0 is the Nusselt number and Pr – the Prandthl number.

Figure 2 presents the algorithm that calculates the droplet diameter evolution, the temperature at the surface of the droplet, the mass fraction of fuel vapor and the mass-flow rate of vaporization.

In this algorithm, we must first calculate all the physical properties of the liquid phase and the gas phase surrounding the droplet (air + fuel vapor), then calculate the heat and mass transfer numbers to find the intersection point of the curves of these two transfer numbers as a function of the droplet surface temperature for the quasi-stationary case. This last point allows us to directly find the rate of vaporization of the droplet and consequently the evolution of the diameter by the relation of the d^2 law.

$$= \infty, \ r = r_s, \ Y_F^{\infty} = 0, \ Y_F = Y_F^S$$
$$B_M = \frac{Y_F^s}{1 - Y_F^s}$$
(28)

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The fuel mass fraction at the surface can be calculated by the expression given [26]:

$$Y_{\rm Fs} = \frac{1}{1 + \left(\frac{P}{P_{\rm Fs}} - 1\right) \left(\frac{M_{\rm a}}{M_{\rm F}}\right)} \tag{29}$$

where M_a is the molar mass of air, M_F – the molar mass of the fuel, P – the total pressure, and P_{Fs} – the partial pressure of the vapor on the surface of the droplet is obtained by the relation [26]:

$$\ln(P_{\rm sat}) = A + \frac{B}{T_{\rm s} - C} \tag{30}$$

where *A*, *B*, and *C* are constants obtained from thermodynamic tables We can also use the formula [26]:

$$P_{\text{sat}} = P_{\text{amb}} \exp\left[\frac{L_{\text{vap}}M}{R} \left(\frac{1}{T_{\text{eb}}} + \frac{1}{T_{\text{s}}}\right)\right]$$
(31)

Heat transfer number

$$B_T = \frac{C_{p_s} \left(T_{\infty} - T_s \right)}{L_{\text{vap}}}$$
(32)

The latent heat is determined by the Watson relation [26]:

$$L_{\rm vap} = L_{\rm vap} T_{\rm eb} \left(\frac{T_{\rm cr} - T_{\rm s}}{T_{\rm cr} - T_{\rm eb}} \right)^{0.38}$$
(33)

where L_{vapTeb} , T_{cr} and T_{eb} are, respectively the heat latent at the boiling temperature, the critical temperature and fuel boiling temperature

Initial parameters and conditions

We assume here the simplest case of a droplet of *n*-heptane initially with a diameter $D_0 = 0.8$ mm. The droplet is placed in the first case in stagnant environment at different temperatures (471 K, 555 K, and 771 K), then in a convective environment at different Reynolds numbers (Re = 5, Re = 20, and Re = 100) at environment temperature T = 300 K. The fuel droplet thermo-physical properties are shown in tab. 1. All thermodynamic properties of the gas are calculated at the reference temperature, the 1/3 rule is used:

$$T_{\rm r} = T_{\rm s} + \frac{T_{\infty} - T_{\rm s}}{3} \tag{34}$$

$$Y_{\rm Fr} = Y_{\rm Fs} + \frac{Y_{\rm F\infty} - Y_{\rm Fs}}{3}$$
(35)

Table 1.	. Fuel	droplet	thermo-p	ohysical	properties
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Fuel droplet property	<i>M</i> [g]	$L_{vap}T_{eb}$ [kJkg ⁻¹]	<i>T</i> _{eb} [°C]	$T_{\rm cr} [^{\circ}{ m C}]$	ρ [kgm ⁻³]	$\lambda [\mathrm{Wm}^{-1}\mathrm{K}^{-1}]$	$C_{p,l}[\mathrm{kJkg}^{-1}\mathrm{K}^{-1}]$
<i>n</i> -heptane	100.198	31.8	371	540	684	0.129	2.23

Results and discussions

We investigate in this work the effect of the Reynolds and Lewis numbers on the droplet vaporization of *n*-heptane in different ambient temperatures 471 K, 555 K, and 771 K and at atmospheric pressure of 0.1 MPa. The analysis carried out here was based on the analytical solution for the governing equations of the vaporization process by calculating the droplet diameter evolution, the temperature at the surface of the droplet, the mass fraction of fuel vapor and the mass-flow rate.

Figure 3 shows the temperature profiles at the droplet surface for different ambient temperatures 471 K, 555 K, and 771 K and at atmospheric pressure of 0.1 MPa. The results are obtained by the theoretical model. The temperature at the droplet surface depends strongly to the ambient temperature that increases proportionally with the environment temperature; the profiles of the temperature at the droplet surface increases linearly for the first time and become constant in the final time to establish at the equilibrium ambient temperature.

Figure 4 shows the evolution of the mass fraction at the surface of the droplet of *n*-heptane as a function of time for different ambient temperatures 471 K, 555 K, and 771 K. The profiles of the mass fraction are almost identical for the three different ambient temperatures with a small variation do to the small vaporization mass-flow rate (0-1.6 10^{-6} g/s). The profiles of the mass fraction at the droplet surface increases linearly in the first time like the profiles of the droplet surface temperature and become constant in the final time until the end of vaporization.



Figures 5-7 show the variation of the normalized squared diameter of the *n*-heptane droplet for different ambient temperatures 471 K, 555 K and 771 K. The variation of the normalized squared diameter of the droplet presents almost linear decreasing evolution as function of time. In these figures the regression of the diameter is faster for the case of temperature 771 K, the results obtained by the theoretical model are almost in good agreement with the experimental data obtained by Hiroshi *et al.* [6].

Figure 8 shows the evolution of the mass-flow rate of vaporization profiles at different ambient temperatures 471 K, 555 K, and 771 K. The profiles of the mass-flow rate has two distinct phases, the first phase has a ascending vaporization rate which increases to the maximum value, the second phase has a decreasing vaporization rate which decreases to the minimum value (end of vaporization) the increases and decreases vaporization rate are very quickly for a higher environment temperature and less for the lower environment temperature. The peak of the vaporization rate is maximum for the higher temperature of 771 K, because the fuel becomes more volatile.

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number to the droplet diameter variation ($D_0 = 0.8$ mm)

Figure 10. Effect of the Reynolds number to the mass-flow rate vaporization ($D_0 = 0.8$ mm)

Figures 9 and 10 shows the effect of the Reynolds number on the droplet diameter variation and the mass-flow rate vaporization profiles, respectively at ambient temperature 300 K. The variation of the normalized squared diameter of the droplet for the case Re = 0presents a low decreasing and linear evolution compared to the other cases and the mass-flow rate of vaporization profiles is low and relatively long. In the case where the Reynolds numbers

varied between 5-100 the regression of the droplet diameter becomes significant and the massflow rate of vaporization increase with the increasing of the Reynolds number.

Figures 11 and 12 shows the effect of the Lewis number to the droplet diameter variation and the mass-flow rate vaporization profiles, respectively for the ambient temperature 300 K. The Lewis numbers varied between 0.8 and 1.2. We observe in these figures that the effect of the Lewis number begins from the phase of decreasing mass-flow rate of vaporization from the time of 20 seconds for our case study. It is observed that when the Lewis number is low less than 1 (Le < 1) the regression of the normalized squared diameter of the droplet is relatively low compared to the case where the Lewis number equal to unity. When the Lewis number is greater than 1 (Le > 1) the diameter regression increases slightly and the mass-flow rate present a short time of vaporization.



Conclusion

In this study we present the effect of the Reynolds and Lewis numbers on the vaporization of liquid fuel droplets and the mass-flow rate vaporization. The results indicate that the variation of the droplet diameter normalized by the initial droplet diameter for the case Re = 0 presents an almost linear and low decreasing evolution compared to the other cases and the profile of the vaporization mass-flow rate presents a long time duration. In the case where the Reynolds numbers varied between 5 and 100, the regression of the droplet diameter is very quickly and the mass-flow rate vaporization increase with the increasing of the Reynolds number. The effect of the Lewis number begins from the phase of decreasing mass-flow rate of vaporization from the time of 20 seconds for our case study. When the Lewis number is low less than 1 (Le < 1), the regression of the droplet diameter normalized by the initial droplet diameter as function of time is low compared to the case where the Lewis number equal to unity. When the Lewis number is greater than 1 (Le > 1) the droplet diameter regression increases slightly.

Nomenclature

- B_M mass transfer number [–]
- B_T heat transfer number [–]
- $C_{p_{g}}$ heat capacity of gas [Jkg⁻¹K⁻¹]
- D° droplet diameter [m]
- $D_{\rm m}$ molecular diffusivity [m²s⁻¹]
- K vaporization rate [m²s⁻¹]
- Le Lewis number [–]
- $L_{\rm vap}$ specific latent heat vaporization [Jkg⁻¹]
- $M_{\rm a}$ air Molar mass [kg]
- $M_{\rm F}~-{
 m fuel}~{
 m Molar}~{
 m mass}~[{
 m kg}]$

- \dot{m} vaporization mass-flow rate [kgs⁻¹]
- Nu Nusselt number [-]
- P pressure [Nm⁻²]
- $P_{\rm Fs}$ saturated vapor pressure [Nm⁻²]
- Pr Prandth Number [–]
- r droplet radius [m]
- Re_d Reynolds number [–]
- Sh₀ Sharwood Number [–]
- $Y_{\rm a}$ air mass fraction [–]
- $Y_{\rm F}$ fuel mass fraction [–]

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- Sc Schmidt number [–]
- *t* time [sesond]
- T temperature [K]
- $T_{\rm eb}$ boiling temperature [K]
- T^{s} surface temperature [K]
- $T_{\rm cr}$ critical point temperature [K]
- $T_{\rm g}$ gas temperature [K]
- $U_{\rm g}$ velocity of the ambient

- $U_{\rm d}$ velocity of the droplet
- u relative velocity [ms⁻¹]

Greek symbols

- η kinematic viscosity [m²s⁻¹]
- λ thermal conductivity [Wm⁻¹K⁻¹]
- $\rho_{\rm g}$ gas density [kgm⁻³]
- $\rho_{\rm L}$ liquid density [kgm⁻³]

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