A turbulent Eulerian multi-fluid reactive flow model and its application in modelling sorption enhanced steam methane reforming

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Abstract. A turbulent multi-fluid reactive fluid model is presented in the paper, which is a combination of a kinetic theory granular flow multi-fluid model (Chao et al., 2011) and the reaction kinetics description (Lindborg, 2008). A two dimensional in-house code was developed to simulate the gas-catalyst-sorbent three-phase reactive flow in the sorption enhanced steam methane reforming fluidized bed reactor. In the simulation, Ca-based sorbents and Ni/MgAl\(_2\)O\(_3\) catalysts are used. The simulation results show that a high production of hydrogen in SE-SMR is obtained compared with the conventional SMR process. The increase of the gas fluidization velocity does not affect the purity of the product hydrogen apparently, while it can shorten the time to get to the breakthrough apparently. The increase of the steam/carbon ratio can increase the purity of the product hydrogen. A homogeneous gas temperature distribution is found which is due to the gas, particle turbulent flows and the heat balance of the SMR-CO\(_2\) adsorption reactions. These simulation results are in good agreement with the experimental results from Johnsen et al. (2006a).

1. Introduction

Hydrogen is currently an important raw material in a number of chemical-, petroleum- and metallurgical processes. It is also considered to be a potential clean energy source (Lindborg, 2008). Currently the large scale production of hydrogen is mainly dominated by steam reforming of fossil fuels. Steam methane reforming (SMR) is an important process for the production of hydrogen in the gas industry. The main reactions for SMR are:

\[
\begin{align*}
CH_4(g) + H_2O(g) &= CO(g) + 3H_2(g) \quad \Delta H_{298} = 206.2 \text{kJ/mol} \quad (I) \\
CO(g) + H_2O(g) &= CO_2(g) + H_2(g) \quad \Delta H_{298} = -41.5 \text{kJ/mol} \quad (II) \\
CH_4(g) + 2H_2O(g) &= CO_2(g) + 4H_2(g) \quad \Delta H_{298} = 164.7 \text{kJ/mol} \quad (III)
\end{align*}
\]

The SMR is normally carried out at 800-900\(^0\)C and 15-30 bars (Johnsen et al., 2006a). The hydrogen and CO\(_2\) are the main products of the SMR process. As the increasing impact of global
warming caused mostly by the increasing concentrations of greenhouse gases, the emission control of CO\textsubscript{2} as the most important greenhouse gas has been concerned by many researchers. So a process called sorption enhanced steam methane reforming (SE-SMR) which is the integration of the hydrogen production and CO\textsubscript{2} separation is becoming important. In this process, carbon dioxide is captured by an on-line sorbent, and the chemical equilibrium is shifted to the product side of the SMR reaction. Therefore, the higher hydrogen production may be obtained. The other advantages are that the reactor could be run at lower temperature (about 600°C) and lower pressure (1-10bars) (Hufton et al., 1999). In the application, the catalysts and sorbents could be either made together in one type of particles, or separately into two types of particles with different properties. The reactor could be either fixed bed or fluidized bed. The focus of the present paper is the binary catalyst-sorbent fluidized bed reactor. In this field, Johnsen et al. (2006a) has investigated the reforming and sorbent calcination in a cyclic operation in a bubbling fluidized bed reactor experimentally. Johnsen et al. (2006b) modelled the SE-SMR and sorbent regeneration processes conducted continuously in two coupled bubbling beds by use of a plug flow model. The objective of the present paper is to establish a more rigorous hydrodynamic multi-fluid reactive flow model, and investigate the reactive flow in the fluidized bed reactor with the binary particles.

2. Model Description

The basic KTGF multi-fluid Eulerian-Eulerian model which was originally reported in a previous publication (Chao et al., 2011) is used in the present study for the gas-solid flow modelling. The reaction kinetics (Lindborg, 2008) is added to the model to simulate the SE-SMR reactions. In the whole paper, digital subscripts are used to identify the fluids. 0 indicates the gas, 1 indicates the catalyst particles, and 2 indicates the sorbent particles.

The continuity equations for the gas and particles are:

\[ \frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i) = \Gamma_i \]  

(IV)

The momentum equation for the gas are:

\[ \frac{\partial}{\partial t}(\alpha_0 \rho_0 \mathbf{v}_0) + \nabla \cdot (\alpha_0 \rho_0 \mathbf{v}_0 \mathbf{v}_0) = -\alpha_0 \nabla p_0 - \nabla \cdot (\alpha_0 \mathbf{r}_0 + \mathbf{r}_t) + \sum_{k=1}^{2} \beta_{0k} (\mathbf{v}_k - \mathbf{v}_0) + \alpha_0 \rho_0 \mathbf{g} \]  

(V)

The momentum equations for the particles are:

\[ \frac{\partial}{\partial t}(\alpha_i \rho_i \mathbf{v}_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i \mathbf{v}_i) = -\alpha_i \nabla p_0 - \nabla \cdot \mathbf{p}_i + \beta_{0i} (\mathbf{v}_0 - \mathbf{v}_i) + \sum_{k=1}^{2} \beta_{ik} (\mathbf{v}_k - \mathbf{v}_i) + \alpha_i \rho_i \mathbf{g} \]  

(VI)

The granular temperature equation for the particles are:

\[ \frac{3}{2} \frac{\partial}{\partial t} (\alpha_i \rho_i \Theta_i) + \frac{3}{2} \nabla \cdot (\alpha_i \rho_i \Theta_i \mathbf{v}_i) = -\mathbf{p}_i : \nabla \mathbf{v}_i - \nabla \cdot \mathbf{q}_i + 3 \beta_{0i} \Theta_i + \gamma_i \]  

(VII)

The equation for the gas turbulent kinetic energy is:

\[ \frac{\partial}{\partial t}(\alpha_0 \rho_0 k_0) + \nabla \cdot (\alpha_0 \rho_0 k_0 \mathbf{v}_0) = \alpha_0 (-\mathbf{r}_t : \nabla \mathbf{v}_0 + S_t) + \nabla \cdot (\alpha_0 \frac{\mu_0^t}{\sigma_0} \nabla k_0) - \alpha_0 \rho_0 \varepsilon_0 \]  

(VIII)
The turbulent energy dissipation rate equation is:

$$\frac{\partial}{\partial t}(\alpha_0 \rho_0 \varepsilon_0) + \nabla \cdot (\alpha_0 \rho_0 \varepsilon_0 \mathbf{v}_0) = \alpha_0 C_1 \frac{\varepsilon_0}{k_0} (-\tau_l : \nabla \mathbf{v}_0 + S_t) + \nabla \cdot \left( \alpha_0 \frac{\mu'_0}{\sigma_e} \nabla \varepsilon_0 \right) - \alpha_0 \rho_0 C_2 \frac{\varepsilon_0^2}{k_0} \tag{IX}$$

The gas temperature transport equation is:

$$\alpha_0 \rho_0 C_{p,0} \frac{DT_0}{Dt} = \nabla \cdot \alpha_0 \lambda_0^{eff} \nabla T_0 + Q_{01} + Q_{02} \tag{X}$$

The catalysts temperature transport equation is:

$$\alpha_1 \rho_1 C_{p,1} \frac{DT_1}{Dt} = \nabla \cdot \alpha_1 \lambda_1^{eff} \nabla T_1 + \sum_{j=1}^{3} R_j^{SMR} \Delta H_j^{SMR} - Q_{01} \tag{XI}$$

The sorbent temperature transport equation is:

$$\alpha_2 \rho_2 C_{p,2} \frac{DT_2}{Dt} = \nabla \cdot \alpha_2 \lambda_2^{eff} \nabla T_2 + R_j^{Sorb} \Delta H_j^{Sorb} - Q_{02} \tag{XII}$$

The gas species transport equations are:

$$\frac{\partial}{\partial t} \left( \rho_0 \omega_j \right) + \nabla \cdot \left( \rho_0 \mathbf{v}_0 \omega_j \right) = \nabla \cdot \left( \rho_0 D_0^{eff} \nabla \omega_j \right) + R_j + \frac{\Gamma_0}{\alpha_0} \omega_j \tag{XIII}$$

The gas shear stress tensor is modelled by:

$$\tau_0 = -2\mu_0 \mathbf{S}_0 \tag{XIV}$$

Where the standard deformation strain is:

$$\mathbf{S}_i = \frac{1}{2} \left( \nabla \mathbf{v}_i + (\nabla \mathbf{v}_i)^T \right) - \frac{1}{3} (\nabla \cdot \mathbf{v}_i) \mathbf{I} \tag{XV}$$

The pressure tensor for the particles of type i includes three parts: the kinetic pressure tensor due to the translational motion of particles, the collisional pressure tensor due to the particle collisions and the friction pressure tensor due to the particle-particle sliding and rolling contact in a dense condition.

$$\mathbf{p}_i = \mathbf{p}_i^{kin} + \mathbf{p}_i^{col} + \mathbf{p}_i^{fri} \tag{XVI}$$

The kinetic pressure tensor for the particles of type i is:

$$\mathbf{p}_i^{kin} = \alpha_i \rho_i^{kin} \mathbf{I} - 2\alpha_i \mu_i^{kin} \mathbf{S}_i \tag{XVII}$$

Where the kinetic pressure for the particles of type i is:

$$p_i^{kin} = \rho_i \Theta_i \tag{XVIII}$$
The kinetic viscosity for the particles of type $i$ is:

$$
\nu_{ki}^{\text{kin}} = \frac{2\mu_{ki}^{\text{dilute}}(1 + 0.8 \sum_{k=1}^{2} \alpha_k (1 + e_{ik}) g_{ik})^2}{0.5 \sum_{k=1}^{2}(1 + e_{ik}) g_{ik}} \quad (XIX)
$$

Where the dilute kinetic viscosity derived using the free path theory is given by:

$$
\mu_{ki}^{\text{dilute}} = \frac{4\rho_i \Theta_i}{\sum_{k=1}^{2} \pi \sqrt{2 \pi d_{ik}^2 n_k} (\Theta_i^{0.5} + \Theta_k^{0.5} - 0.56 \Theta_i^{0.25} \Theta_k^{0.25})} \quad (XX)
$$

The collisional pressure tensor is:

$$
P_i^{\text{col}} = \alpha_i \mu_i^{\text{col}} I - \sum_{k=1}^{2} \alpha_i (2 \mu_i^{\text{col}} S_i + \mu_i^{\text{col}, B} \nabla \cdot v_i I + 2 \mu_i^{\text{col}} S_k + \mu_k^{\text{col}, B} \nabla \cdot v_k I) \quad (XXI)
$$

The collisional particle pressure is:

$$
p_i^{\text{col}} = \sum_{k=1}^{2} d_{ik}^3 g_{ik} (1 + e_{ik}) \frac{\pi \alpha_k \rho_i \rho_k}{3(m_i + m_k)} (\Theta_i + \Theta_k) \quad (XXII)
$$

The particle viscosities are:

$$
\mu_i^{\text{col}} = \frac{\sqrt{2\pi \alpha_k \rho_i \rho_k}}{72(m_i + m_k)} (1 + e_{ik}) g_{ik} d_{ik}^3 (4 \Theta_i^{0.5} + 3 \Theta_k^{0.5} - 1.9550 \Theta_i^{0.25} \Theta_k^{0.25}) \quad (XXIII)
$$

The bulk particle viscosities equal to the double of the corresponding collisional viscosities.

$$
\mu_i^{\text{col}, B} = 2 \mu_i^{\text{col}} \quad (XXIV)
$$

The collisional particle pressure is:

$$
P_i^{fri} = \alpha_i p_i^{fri} I - 2\alpha_i \mu_i^{fri} S_i \quad (XXV)
$$

Where the friction pressure is:

$$
p_i^{fri} = \begin{cases} 
\frac{\zeta (\alpha_1 + \alpha_2 - \alpha_{\min})}{(\alpha_1 + \alpha_2)(\alpha_{\min} - \alpha_1 - \alpha_2)^2} & \text{if } \alpha_1 + \alpha_2 > \alpha_{\min} \\
0 & \text{if } \alpha_1 + \alpha_2 \leq \alpha_{\min}
\end{cases} \quad (XXVI)
$$

The friction viscosity is given by:

$$
\mu_i^{fri} = \frac{\sqrt{2} p_i^{fri} \sin \varphi}{2 \alpha_i \sqrt{S_i : S_i + \Theta_i / d_i^2}} \quad (XXVII)
$$

Please refer to the literature (Lindborg, 2008) for the basic parameters in the friction stress and viscosity models. The granular heat flux contains two parts: the kinetic and collisional contributions.
\[ q_i = q_i^{\text{kin}} + q_i^{\text{col}} \]

The kinetic part is:
\[ q_i^{\text{kin}} = -\alpha_k q_i^{\text{kin}} \nabla \Theta_i \]

The collisional part is:
\[ q_i^{\text{col}} = -\alpha_k q_i^{\text{col}} \nabla \Theta_i \]

Where the kinetic and collisional heat conductivities are:
\[ k_i^{\text{kin}} = \frac{2k_i^{\text{dilute}}}{0.5} \left[ 1 + 1.2 \sum_{k=1}^{2} \alpha_k (1 + e_{ik}) g_{ik} \right] \]

\[ k_i^{\text{col}} = \left( \frac{2\pi\alpha_k \rho_k}{5(m_i + m_k)} (1 + e_{ik}) g_{ik} d_{ik}^4 \right) \sqrt{\Theta_i} \]

Where the dilute heat conductivity is:
\[ k_i^{\text{dilute}} = \frac{15}{4} \mu_i^{\text{dilute}} \]

The source term for the granular temperature equations are:
\[ \gamma_i = \sum_{k=1}^{2} \frac{\pi c_{ik}^2 - 1}{8(m_i + m_k)} \left( 6.38(\Theta_i^{1.5} + \Theta_k^{1.5}) + 1.98(\Theta_i^{0.5} + \Theta_k^{0.5} \Theta_k) \right) \]

\[ + \sum_{k=1}^{2} \frac{2\pi}{60} d_{ik}^3 g_{ik} m_i m_k m_i n_k n_k (1 - e_{ik}^2) \left( \nabla \cdot v_k (15\Theta_i + 9\Theta_k) + \nabla \cdot v_k (15\Theta_k + 9\Theta_i) \right) \]

The gas particle drag is given by:
\[ \beta_{0k} = \begin{cases} 
\frac{15\rho_0 (1 - \alpha_0) a_k}{a_0 d_k^2} + \frac{1.75 \alpha_k \rho_0 |v_0 - v_k|}{d_k} & \text{if } \alpha_0 \leq 0.8 \\
\frac{3C_D \alpha_0 \rho_0 |v_0 - v_k|}{4d_k} - 1.65 & \text{if } \alpha_0 > 0.8 
\end{cases} \]

Where the coefficient \( C_D \) is:
\[ C_D = \begin{cases} 
\frac{24}{Re_k} [1 + 0.15(Re_k)^{0.687}] & \text{if } Re_k < 1000 \\
0.44 & \text{if } Re_k \geq 1000 
\end{cases} \]

Where the particle Reynolds number for the particles of type k is:
\[ Re_k = \frac{\alpha_0 d_k \rho_0 |v_0 - v_k|}{\mu_0} \]

The particle-particle drag which considers both the kinetic and collisional effects is:
The Reynolds stress $\tau_t$ is modelled using the gradient- and Boussinesq approximations:

$$\tau_t = -2\mu_0^t S_0 + \frac{2}{3} \rho_0 k_0 I$$  \hspace{1cm} (XXXIX)

Where the dynamic turbulent viscosity $\mu_0^t$ is expressed by:

$$\mu_0^t = \rho_0 C_\mu \frac{k_0^2}{\varepsilon_0}$$  \hspace{1cm} (XL)

The turbulent source term due to the existence of the particles is (Lindborg, 2008):

$$S_t = C_b \beta_{01} (v_1 - v_0)^2 + C_b \beta_{02} (v_2 - v_0)^2$$  \hspace{1cm} (XLI)

Please refer to the literature (Chao et al., 2011) for the empirical parameters of the K-Epsilon model. Please refer to Lindborg (2008) for the expressions about the effective heat conductivities $\lambda_{ij}^e$, the effective diffusion coefficient $D_0^{eff}$ and the interfacial species transfer $\omega_j^t$.

The SMR reaction kinetics from Xu and Froment (1989) is used here:

$$R_1^{SMR} = \frac{k_1}{p_{H_2}^{1.5}} \left[ \frac{p_{CH_4} p_{H_2} O - p_{H_2}^3 p_{CO}/K_1}{DEN^2} \right]$$  \hspace{1cm} (XLII)

$$R_2^{SMR} = \frac{k_2}{p_{H_2}} \left[ \frac{p_{CO} p_{H_2} O - p_{H_2} p_{CO}/K_2}{DEN^2} \right]$$  \hspace{1cm} (XLIII)

$$R_3^{SMR} = \frac{k_3}{p_{H_2}^{1.5}} \left[ \frac{p_{CH_4}^2 p_{H_2} O - p_{H_2}^4 p_{CO_2}/K_3}{DEN^2} \right]$$  \hspace{1cm} (XLIV)

where

$$DEN = 1 + K_{CO pCO} + K_{H_2} p_{H_2} + K_{CH_4} p_{CH_4} + K_{H_2 O pH_2 O} / p_{H_2}$$  \hspace{1cm} (XLV)

$R_1, R_2, R_3$ correspond to the reactions (I), (II) and (III), respectively. Please refer to Xu and Froment (1989) for the different lower case and caps k and K parameters.

The rate equation for $CO_2$ adsorption by the CaO sorbent is taken from Sun et al. (2008):

$$CO_2(g) + CaO(s) = CaCO_3(s) \hspace{1cm} \Delta H_{298} = -178 \text{ kJ/mol}$$  \hspace{1cm} (XLVI)

$$R^{Sorb} = 56 k_s (1 - X) (p_{CO_2} - p_{CO_2,eq})^n S$$  \hspace{1cm} (XLVII)

Where $n$ equals 1 when $(p_{CO_2} - p_{CO_2,eq}) \leq 10 KPa$, and 0 when $(p_{CO_2} - p_{CO_2,eq}) > 10 KPa$. The coefficient $k_s$ is taken from Sun et al. (2008). The equilibrium pressure of $CO_2$ is given by (Sun et al., 2008):

$$P_{CO_2,eq} = 10^{(-8308/T_2 + 9.079)}$$  \hspace{1cm} (XLVIII)
3. Model application and results

A SE-SMR process is investigated. The basic simulation parameters are shown in 1. In the investigations, the initial densities and particle diameter for the binary particles are assumed same. The binary particles are well mixed initially.

Figure 1 shows the comparison of the average outlet hydrogen concentration for SMR and SE-SMR processes. The outlet hydrogen purity at the SE-SMR process is much higher than the SMR process. The adsorption of CO$_2$ shifted the reaction apparently. When the outlet pressure is increased, the hydrogen purity is decreased, especially for the SMR process.

| Parameter                      | value                          |
|--------------------------------|--------------------------------|
| Reactor size                   | L=4m,D=0.3m                    |
| Packed bed height              | 1.5m                           |
| Sorbent/catalyst ratio         | 5                              |
| Initial total particle volume fraction | 0.58                          |
| Sorbent, catalyst density      | 1500kg/m$^3$                   |
| Sorbent, catalyst particle size| 500$\mu$m                      |
| Outlet gas pressure            | 1bar,10bar                     |
| Grids                          | 30$\times$80                   |
| Gas fluidization velocity      | 0.4m/s,0.6m/s,0.8m              |
| Restitution coefficient of particles | 0.999                        |
| Steam-to-carbon feed molar ratio | 3,4,5                         |
| Inlet temperature              | 848K                           |

Figure 1. The comparison of the average outlet concentration of hydrogen for SMR and SE-SMR at different pressures.

(gas fluidization velocity $v_0 = 0.4m/s$, steam to carbon molar ratio $r_{sc} = 5$)

The gas fluidization velocity is a very important parameter to decide the flow behavior of the fluidized beds, and the residence time of the gas. An increase of the gas velocity also means an increase of the gas treatment per unit time. Figure 2 shows that the outlet hydrogen concentration does not vary apparently with an increase of the gas velocity. But the increase of the gas velocity can shorten the time to get to the breakthrough greatly. So in a real application, a higher gas treatment capacity requires a matched corresponding sorbent regeneration and re-injection rate in order to obtain a steady and continuous performance.
The influence of the gas fluidization velocity on the outlet average product hydrogen concentration for a SM-SMR process.

( steam to carbon molar ratio \( r_{sc} = 5 \), outlet pressure \( p = 1\text{bar} \) )

The influence of the steam carbon ratio in the SMR process is very important because this ratio can shift the reactions (I), (II) and (III) to the right hand side. The influence of this ratio on the SE-SMR reactions are shown in Figure 3. An increase of this ratio can lead to a comparatively higher product hydrogen purity. Compared with the increase of this ratio from 4 to 5, the increase from 3 to 4 is more economically efficient.

The temperature distribution is very important because the reaction rates with regard to the reactions (I), (II) and (III) and (XLVI) are all temperature dependent. Figure 4 shows the average axial temperature distribution. The variations are very small. The main reasons for this trend are that the released heat by \( CO_2 \) adsorption is close to the absorbed heat by

Figure 2. The influence of the gas fluidization velocity on the outlet average product hydrogen concentration for a SM-SMR process.

( gas fluidization velocity \( v_0 = 0.4\text{m/s} \), outlet pressure \( p = 1\text{bar} \) )

Figure 3. The influence of the steam carbon ratio on the SE-SMR reactions are shown in Figure 3. An increase of this ratio can lead to a comparatively higher product hydrogen purity. Compared with the increase of this ratio from 4 to 5, the increase from 3 to 4 is more economically efficient.

Figure 4. Gas temperature distribution.

(steam to carbon molar ratio \( r_{sc} = 5 \), gas fluidization velocity \( v_0 = 0.4\text{m/s} \), outlet pressure \( p = 1\text{bar} \) )
methane reforming, and that the gas and solid phases in the bubbling bed are well-mixed due to the turbulent flow. Figure 5 shows the sorbents volume fraction fluctuations at $z=1m$ in the center of bed. The fraction varies dramatically with time, it is an results of the gas and particle turbulent flow. The turbulent flows make the fluidized bed has homogeneous temperature distribution, which is an apparent advantage compared with the fixed bed reactor (Lindborg, 2008). These simulation results generally fit well with the experimental results from Johnsen et al. (2006a).

4. Conclusions

A turbulent multi-fluid reactive fluid model has been presented, and applied in modelling a sorption enhanced steam methane reforming process. The simulation results show that a high production of hydrogen in SE-SMR is obtained compared with the conventional SMR process. The increase of the gas fluidization velocity does not affect the purity of the product hydrogen apparently, while it can shorten the time to get to the breakthrough dramatically. The increase of the steam/carbon ratio can lead to a purity increase of the product hydrogen. The temperature in the fluidized bed is homogeneous which is a result of the gas and particle turbulent flows and the heat balance of the SMR and $CO_2$ adsorption reactions.

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6. Notation

$C_{p,k}$ heat capacity of phase $k$.
$d$ particle diameter, $m$.
$D, L$ reactor diameter and length, $m$.
$e$ restitution coefficient of particles.
$g$ gravity constant, $m^2/s^2$.
$H$ enthalpy, $J/kmol$.
$k_0$ gas turbulent kinetic energy, $m^2/s^2$.
$k_{col}^i$ collisional heat conductivity, $Pas$.
$k_{kin}^i$ kinetic heat conductivity, $Pas$. 

Figure 5. Sorbents volume fraction fluctuations at one point of the reactor.
(steam to carbon molar ratio $r_{sc} = 5$, gas fluidization velocity $v_0 = 0.4m/s$, outlet pressure $p = 1bar$)
mass, kg.

pressure, Pa.

the heat transferred between the gas and particle i, $J/(m^3s)$.

reaction rate, $kg/(m^3s)$.

pressure tensor, Pa.

temperature, K.

velocity, $m/s$.

Conversion.

volume fraction.

density, $kg/m^3$.

rate of mass transfer, $kg/(m^3s)$.

drag coefficient, $kg/(m^3s)$.

granular temperature, $m^2/s^2$.

gas stress tensor.

viscosity, Pa.s.

turbulent energy dissipation rate, $m^2/s^3$.

effective thermal conductivity, $J/(msK)$.

molar fraction of gas species j.

indications of particles of type i and k.

collisional, kinetic and frictional separately.

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