Comparison of an Optimal Stomatal Regulation Model and a Biochemical Model in Explaining CO_2 Exchange in Field Conditions

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Gas exchange of *Pinus sylvestris* L. was studied in subarctic field conditions. Aspects on optimal control of the gas exchange were examined using approach by Hari et al. (Tree Phys. 2: 169–175, 1986). Biochemical model by Farquhar et al. (Planta 149: 78–90, 1980) was utilized to describe the photosynthetic production rate of needles. The model parameters were determined from field measurements. The results from the optimization approach and biochemical model were compared and their performance was found quite similar in terms of R^2 calculated using measured exchange rates (0.89 for optimization model and 0.85 for biochemical model). Minor differences were found in relation to responses to intercellular carbon dioxide concentration and temperature.

Keywords photosynthesis, CO_2 exchange, biochemical model, optimization, *Pinus sylvestris* L., Scots pine

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1 Introduction

Models of gas exchange rates of leaves in field conditions are required for ecosystem studies. There exist different approaches which can be utilised to predict exchange rates. Photosynthetic production has been studied in detail by Farquhar et al. (1980) who introduced a biochemical model of photosynthesis. This model allows leaf scale fluxes to be calculated if conductances are known or modelled by other means. Today the model by Farquhar et al. (1980) is widely used for estimations of leaf level gas exchange and further as a submodel in large ecosystem models. Cowan (1977) presented an insight into optimization in gas exchange. Optimal control of the gas exchange of leaves is based on finding the mode of stomatal functioning which leads to minimal loss of water and maximal gain of carbon dioxide. Hari et al. (1986) applied the ideas of optimal control to develop a predictive gas exchange model which also results in the photosynthetic production of leaves.

Comparison of the two approaches, optimal stomatal control and photosynthetic production by a biochemical model, adds a new perspective to the relationships between CO_2 uptake and environment. It is useful to study whether differences in responses of the exchange rate to environmental variables could arise due to different approaches, since the leaf level results may affect larger scenarios. The model parameters are often fitted by utilizing field measurements influenced by varying environmental conditions. It is therefore reasonable to use field measurements also in the comparison of the models.

In this work, the biochemical approach was utilized as a description of the photosynthetic reactions with input information like conductance taken directly from transpiration measurements instead of modelling it. Optimization approach was used in a form where a simple formulation of photosynthetic production, transpiration and conductance were closely linked together and CO_2 assimilation rate and conductance were predicted by the model. Relevant parameters of the biochemical model and optimal stomatal regulation model were determined from field measurements. Gas exchange of *Pinus sylvestris* L. was studied in remote subarctic field conditions in northern Finland using automated measuring system which enabled recording of gas exhange rates of intact shoots at 12 min intervals throughout the growing season. Results of simulated gas exchange rates of Scots pine using both models were compared to the measured rates.

2 Materials and Methods

2.1 Measurement Set-up

Gas exchange rate of Scots pine (*Pinus sylvestris* L.) was registered continuously at 12 min intervals during summer months in the Värriö environmental measuring station (67°46’N, 29°35’E, 390 m a.s.l.). Monitoring was performed using well-established automated cuvette system developed by the personnel on the station and in the University of Helsinki (Hari et al. 1999). The system consisted of trap-like cuvettes, a pneumatic system for controlling cuvettes, gas flow controllers and gas analyzers (Hartmann and Braun URAS 4 infrared absorption analyzers). The system was controlled by a computer.

An intact pine shoot (150–250 needles) was installed inside the ventilated cylindrical acrylplastic cuvette (volume 3.5 dm^3). The lid of the cuvette was closed for only 70 s once every 12 minutes so that the temperature increase during closing stayed in insignificant level and ambient conditions prevailed for most of the time. Cuvette air was mixed with a fan. The change in CO_2 and water vapour concentrations was registered once in every ten seconds while the cuvette was closed and the exchange rates were determined by methods presented in Aalto (1998). During measurements the outgoing sample air and incoming replacement air flows were balanced so that no pressure drop occurred inside the cuvette. The sample was transported to the gas analyzers by heated teflon pipes. There was a constant flow of air through the pipes also between measurements in order to avoid condensation of water and exchange of CO_2 with the walls of the tubing. Calibration and pressure corrections were performed for each measurement. Temperature (CuKo thermoelements) and photosynthetically active radiation PAR (LiCor 190 SB sensors) were measured both inside and outside the cuvette. The cuvettes were installed in unshaded positions in the top of the trees and the shoots consisted of one- and two-year-old needles. The reliable functioning of the system has been confirmed by laboratory and field studies (e.g. Hari et al. 1999). A variety of meteorological and other forest ecological measurements are also performed at the station (Hari et al. 1994, Ahonen et al. 1997).

2.2 Optimal Stomatal Regulation Model (OSRM)

The optimal stomatal regulation model was obtained from Hari et al. (1986) (See also Beninger et al. 1996 and Mäkelä et al. 1996). According to the formulation, CO_2 exchange (A) and transpiration (E) rates depend on stomatal conductance g:

$$A = \frac{g c_a}{g + \alpha I c_i} \alpha I c_i \tag{1}$$

$$E = 1.6 g (w_i - w_a) \tag{2}$$

where c and w are CO_2 and H_2O concentrations (g/m^3) respectively, inside stoma (i) and in ambient air (a). α is an empirical parameter to be fitted from measurements (see Table 1) and I is irradiance. As a solution of the optimization, conductance can be expressed followingly:

$$g = \alpha I c_i \left(\sqrt{\frac{c_a}{1.6\lambda[w_i - w_a]}} - 1 \right) \tag{3}$$

where λ is the 'cost of water' also to be fitted from the measurements. Minimum value of g is restricted to 0 and maximum to g_0 describing the state of fully open stomata.

2.3 Biochemical Model for Photosynthetic CO_2 Assimilation (BPM)

2.3.1 Model Structure

The model used was based on the original idea by Farquhar et al. (1980) as modified by Harley and Baldocchi (1995) and Lloyd et al. (1995). The functional form of the model is identical to Aalto and Juurola (2001), modifications are due to values of the major parameters concerning carbon assimilation ($J_{\max}$, q, Θ and $V_{c(\max)}$) and respiration (R_d) and their temperature dependences.

In short, the net rate of CO_2 exchange is (e.g. Lloyd et al. 1995)

$$A = \min \begin{cases} J \dfrac{(c_i - \Gamma_*)}{4(c_i + 2\Gamma_*)} - Rd \\ V_{c(\max)} \dfrac{(c_i - \Gamma_*)}{k_c(1 + o / k_o) + c_i} - R_d \end{cases} \tag{4}$$

first expression being the RuBP regeneration limited exchange rate and second the net Rubisco-limited rate (c_i in µmol/mol). For more detailed information and numerical values used for Michaelis-Menten constants k_c, k_o and Γ_*, CO_2 compensation point in the absence of mitochondrial respiration, we refer to Aalto and Juurola (2001).

The dependence of J on irradiation can be written as (e.g Lloyd et al. 1995)

$$J = \frac{qI + J_{\max} - \sqrt{(qI + J_{\max})^2 - 4\Theta q I J_{\max}}}{2\Theta} \tag{5}$$

where $J_{\max}$ is the maximum of the electron transport rate, q is the effectivity factor for the use of light and Θ is the convexity factor of the curve.

The following equation was used for $J_{\max}$ (Lloyd et al. 1995, Farquhar et al. 1980):

$$J_{\max} = \frac{B \exp\left[\dfrac{E_j (T / 298.15 - 1)}{RT}\right]}{1 + \exp\left[\dfrac{S_j T - H_j}{RT}\right]} \tag{6}$$

where E_j is activation energy, H_j curvature parameter and S_j temperature response parameter for RuBP-regeneration limited assimilation rate, and B is a constant

$$B = J_{\max,298}\left(1 + \exp\left[\frac{298 S_j - H_j}{298 R}\right]\right) \tag{7}$$

The Arrhenius type of relationship (e.g. Harley and Baldocchi 1995) was utilized for temperature dependences of the maximum carboxylation rate $V_{c(\max)}$ and the rate of non-photorespiratory respiration R_d:

$$f_T = f_{298} \exp\left[\frac{E_f (T - 298.15)}{298.15 RT}\right] \tag{8}$$

where f_T is the value of a given parameter at temperature T and E_f are activation energies. R is the gas constant and T is temperature in K.

2.3.2 Methods of Evaluation

Measurements of shoot gas exchange during August 1997 were utilized in order to evaluate the parameters of the biochemical model. CO_2 and H_2O fluxes, conductances and intercellular CO_2 concentrations were obtained from cuvette measurements as in Aalto (1998). Measurements before noon were selected to attain high conductance conditions.

The irradiance response of the CO_2 flux was modelled using only the expression for RuBP regeneration limited exchange rate (Eq. 4). Additional selection criterion was therefore applied to the research material in order to keep the stomatal concentration of CO_2 (c_i) at high level, i.e ratio of stomatal to ambient concentration was required to exceed 0.5. Also, measurements at PAR values exceeding 600 µmol $m^{-2}s^{-1}$ were abandoned.

The initial slope of the irradiance curve, q (Eq. 5), was solved first keeping Θ constant and focusing on good fit near the irradiance compensation point. The curvature factor Θ was solved using the estimation for q and freely varying $J_{\max}$. The value of q was then re-estimated using the new solution for Θ. Values obtained for q and Θ (Table 1) were then used throughout the work assuming invariability over the temperature range examined (6–20°C). Results were similar to Aalto (1998) using measurements from the same pine stand.

$J_{\max}$ (Eq. 5) was solved using fixed q and Θ. This was done in order to minimize the number of free variables and thus enable studies of the temperature dependence of the parameter. The temperature-induced variation was examined by solving $J_{\max}$ for each four-degree intervals. $J_{\max}$ was found to increase relatively slowly with the temperature. Eq. 6 was fitted to the results for $J_{\max}$ (Table 1). $J_{\max}$ was assumed to be constant above 20°C because there were only few measurement points at high temperatures.

$V_{c(\max)}$ was fitted to before-noon measurements at irradiance levels exceeding 800 µmol $m^{-2}s^{-1}$ using expression for the net Rubisco-limited rate (Eq. 4). The temperature dependence of $V_{c(\max)}$ (at 8–24°C) was solved from Eq. 8 (see Table 1) for four-degree intervals as in $J_{\max}$. $V_{c(\max)}$ was constantly increasing with temperature showing relatively similar results to the ones obtained by Aalto (1998).

Table 1. Values for parameters in model Eqs. 1–8. T is temperature in K. *: $R_{d,298}$ must be divided by 1.45 when irradiance level exceeds 50 µmol $m^{-2}s^{-1}$. $J_{\max}$ was assumed to equal 112 µmol $m^{-2}s^{-1}$ in temperatures higher than 293K.

BCM	
E_j	45 600 J mol^{-1}
S_j	2085 J mol^{-1} K^{-1}
H_j	615 600 J mol^{-1}
B	184 µmol $m^{-2}s^{-1}$
$E_{Vc(\max)}$	50 000 J mol^{-1}
$V_{c(\max),298}$	48 µmol $m^{-2}s^{-1}$
E_{Rd}	45 000 J mol^{-1}
$R_{d,298}$	1.15 µmol $m^{-2}s^{-1}$
q	0.14
Θ	0.7
OSRM	
α	0.0011 m^3 µmol^{-1}
λ	0.012 g(CO_2) / g(H_2O)
g_0	0.002 m s^{-1}

Respiration was solved from measurements during night. Respiration increased with rising temperature (Table 1). Non-photorespiratory respiration in dark was assumed to be suppressed in light by factor 1.45 as suggested by Wang (1996) for Scots pine.

In the case of OSRM (optimal stomatal regulation model) conductance was determined for every measurement from Eq. 3 and the exchange rate of CO_2 from Eq. 1. Measurements during five first days of August were utilized for estimation of α and λ (Table 1) by minimizing the residual sum of squares. Exchange rates during the rest of the month were predicted by the model using the obtained values.

3 Comparison of Models

Proportion of explained variance

$$R^2 = 1 - \Sigma_i (Y_i - Y_{i,est})^2 \,/\, \Sigma_i (Y_i - \overline{Y}_i)^2 \qquad (9)$$

where $Y_{i,est}$ is the modelled and Y_i measured CO_2 flux, was calculated for different cases. When the whole month was examined R^2 was 0.85 for BPM (biochemical model for photosynthetic CO_2 assimilation) and 0.89 for OSRM. Sensitiv-

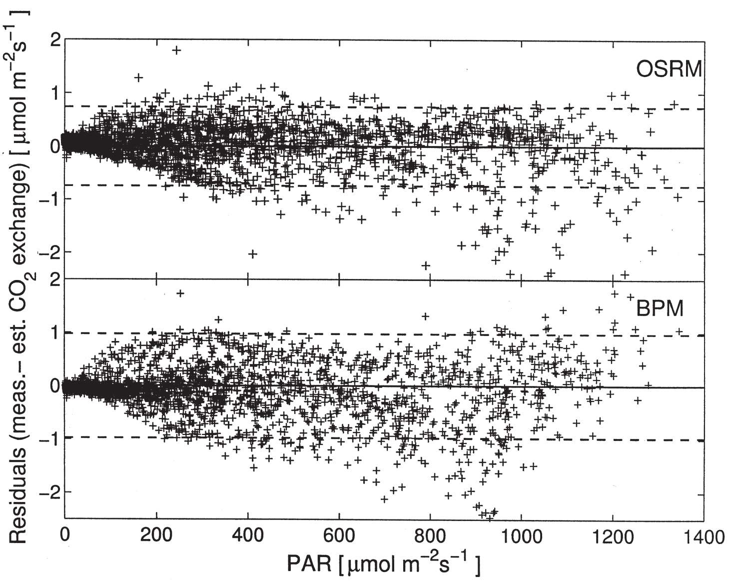

Fig. 1. Residuals (estimated – measured CO_2 exchange rate) as a function of irradiance. 95% of the results lay between dashed lines.

ity analysis revealed only minor changes; when the most important single parameter in the BPM, J_{max}, was increased by 10% the resulting value for R^2 was 0.83. J_{max} was also modified to experience steeper increase with increasing temperature according to earlier results for Scots pine growing in southern Finland (Wang 1996). This resulted in R^2 of 0.83. In comparison to the J_{max} fitted for the northern Scots pine, residuals suggested slightly more overestimations of exchange rates in high temperatures and underestimations in low temperatures.

Residual plot as a function of irradiance (Fig. 1) shows that largest errors according to OSRM occur during very high irradiation levels, while the majority of large errors in BPM is in slightly lower irradiances (it is supposed that these errors are overestimations by the models since the fluxes are positive during daytime when irradiance levels are high). Residuals are rather well centered around zero when the 95% majority is examined. Values during night at low irradiance show moderate overestimation of respiration rate for OSRM and underestimation for BPM (signs opposed).

Temperature plot (Fig. 2) shows largest errors for BPM in higher temperatures than for OSRM. Otherwise the plot is quite evenly scattered. A weak trend can perhaps be observed from overestimations in low temperatures to underestimations in high temperatures for OSRM and vice versa for BPM. This suggests that the function for J_{max} (Eq. 6) in BPM might have given a better fit with even weaker response to increasing temperature.

Plot as a function of c_i (Fig. 3) shows largest errors in the typical mid-range of c_i for daytime CO_2 exchange. On the lowest range of c_i there are some large errors for BPM and during the near-nightime high c_i OSRM produces more scattering which seems to be somewhat clumped. c_i for BPM is deduced directly from measurements using transpiration rates and ambient CO_2 concentration and c_i for OSRM is solved using the optimization scheme.

Studies of diurnal dependence (Fig. 4) show similar decreasing trend to both models. Exchange rates during mornings are slightly underestimated and afternoons overestimated.

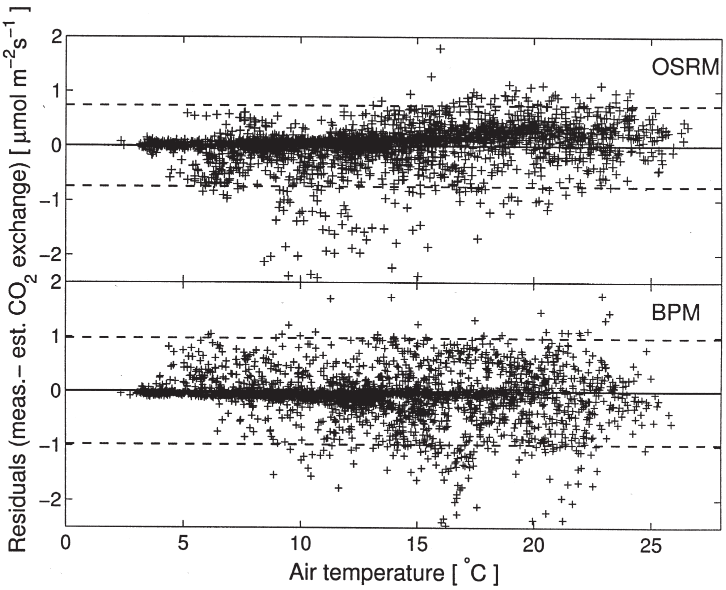

Fig. 2. Residuals (estimated – measured CO$_2$ exchange rate) as a function of temperature. 95% of the results lay between dashed lines.

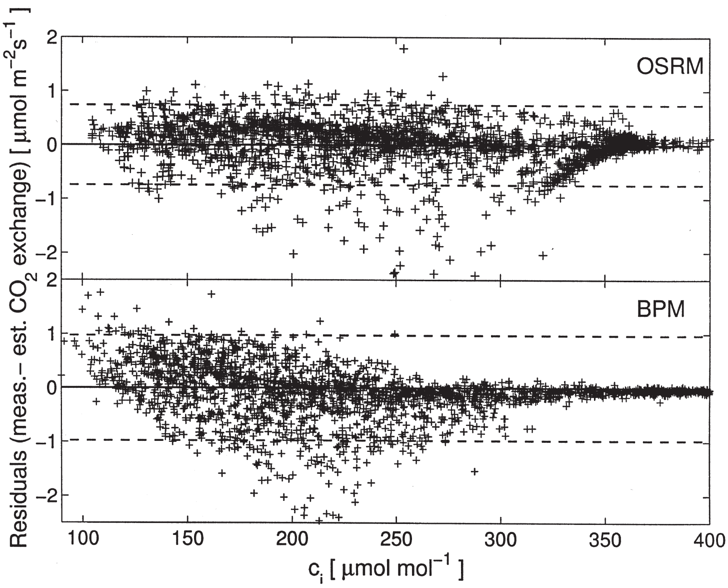

Fig. 3. Residuals (estimated – measured CO$_2$ exchange rate) as a function of intercellular CO$_2$ concentration. 95% of the results lay between dashed lines.

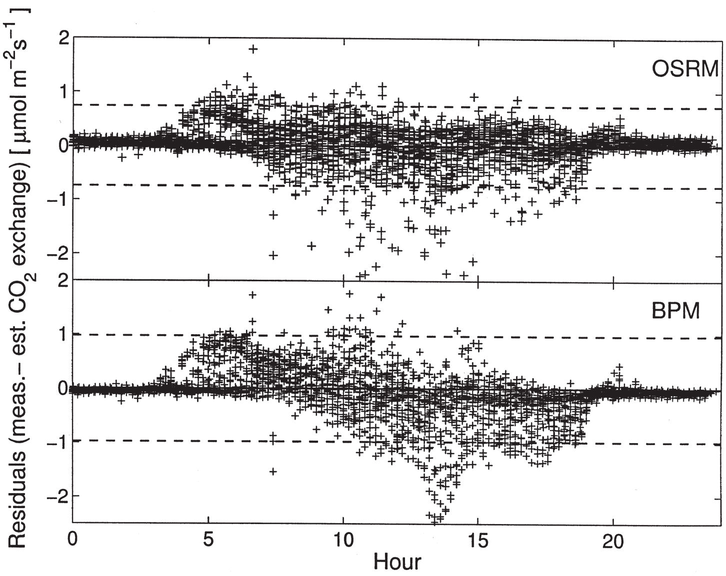

Fig. 4. Diurnal variation of residuals. 95% of the results lay between dashed lines.

4 Discussion

The first cold period after summer occurred in the middle of August (Fig. 5). In general, both models underestimated the exchange rates before the low temperature period and overestimated during late August (Fig. 6) thus suggesting cold-induced changes in the photosynthetic responses of the needles. The minimum diurnal temperatures were 2–4°C during the cold period, but daytime maximum temperatures reached only 6–10°C with simultaneous high irradiation levels.

The largest overestimations by BPM occurred right after the cold period when the daytime temperatures rapidly elevated to over 20°C. During the cold period OSRM overestimated fluxes, while BPM showed slight underestimations during that time. The results are supported by for example Korpilahti (1988) and Hollinger et al. (1999), who reported a drawdown on carbon uptake of a boreal coniferous forest after first autumn frost. Leverenz and Öquist (1987) found a decrease in quantum yields of photosynthesis for Scots pine when temperature decreased below 5°C. The effect was most profound in the middle of the summer and decreased towards autumn.

Some underestimations by BPM occur during extremely low c_i (in the beginning of the month) which indicates specific effects due to the model structure not taking into account possible partial activation of the carboxylase-oxygenase enzyme, as presented by Farquhar and von Caemmerer (1982). In the diurnal pattern these low values are located around midday, while during afternoons overestimations of fluxes are more usual than underestimations.

Generally results are good and rather similar for both approaches OSRM showing slightly higher value for R^2 with current parametrizations. Both models can be used to predict CO_2 exchange of pine needles in northern, relatively cold but humid, environment with sufficient accuracy. However, it has to be noticed that the photosynthetic capacity may change according to canopy height and there exists different approaches to scale from leaf photosynthesis to canopy photosynthesis (de Pury and Farquhar 1997). This study does not take into account those changes and their possible effects to the model comparison result.

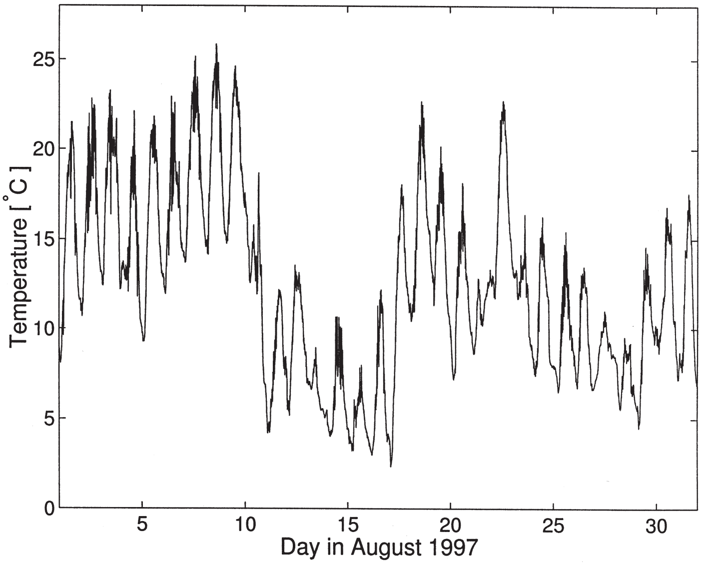

Fig. 5. Ambient temperature during August 1997 in Värriö.

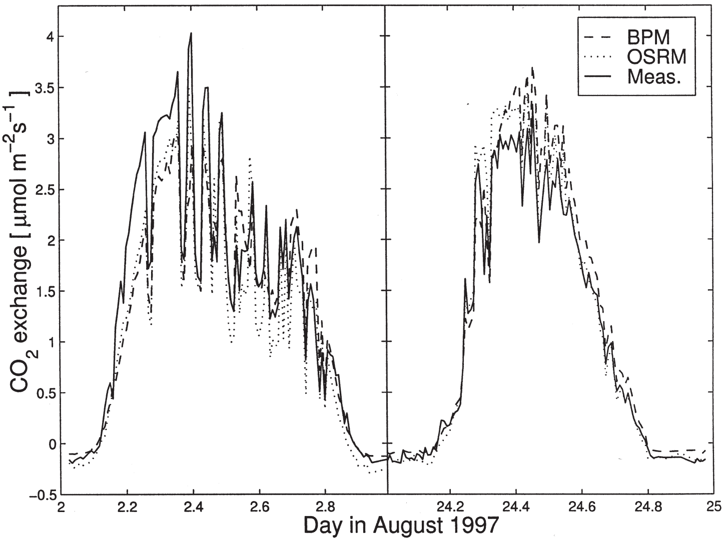

Fig. 6. CO_2 exchange according to optimal stomatal regulation model, biochemical model and measurements before and after cold period in Värriö.

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