

# A kinetic study of the complete oxidation of ethene, propane and their mixtures on a Pd/Al<sub>2</sub>O<sub>3</sub> catalyst

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## Abstract

The complete oxidation of ethene and propane as individual hydrocarbons and of their mixtures on a Pd/Al<sub>2</sub>O<sub>3</sub> catalyst has been studied using an internal recycle reactor. The pressure was varied from 1.6–5 bar and the temperature from 180–220 °C for ethene oxidation and from 280–330 °C for propane oxidation. The maximum hydrocarbon concentration was ca. 3000 ppm or 0.3 vol. %.

The effect of the reaction products and the co-educt on the kinetics was investigated and it is shown that whereas water significantly retards the oxidation, the influence of CO<sub>2</sub> is negligible. Propane oxidation is inhibited by ethene. Such inhibition can only partly be explained by the additional water formed due to the combustion of ethene. The conversions in these experiments studied ranged between 70% and 90% for ethene and between 15% and 30% for propane, respectively.

Four different rate expressions have been tested bearing in mind that the influence of water must be taken into account in any adequate description of the experimental data. The best-fitting rate expression described the experimental data to within an average error of 17% for ethene and 13% for propane, respectively.

A comparison of the results with data from dynamic experiments showed a reasonable agreement.

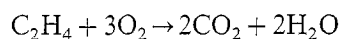
**Keywords:** Kinetic study; Ethene complete oxidation; Propane complete oxidation; Ethene/propane mixtures complete oxidation; Pd/Al<sub>2</sub>O<sub>3</sub> catalyst

## 1. Introduction

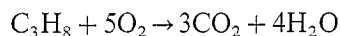
Catalytic combustion can be applied for the destruction of volatile organic compounds (VOCs) in polluted air (see, for example, Prasad *et al.* [1] and Zwinkels *et al.* [2]). Recently several research groups, have studied the behaviour of catalytic after-burners (see, for example, Tichenor and Palazzolo [3], Mazzarino and Barresi [4] and Hermia and Vigneron [5]).

We have studied the catalytic oxidation of VOCs in a number of catalytic packed bed reactors in our laboratory (see Van de Beld *et al.* [6, 7]) with both a.o. ethene and propane being used as sample substances. For the description and prediction of the behaviour of such

reactors, a knowledge of the reaction system is necessary. In this paper, we report on kinetic studies of the complete oxidation of ethene and propane on a Pd/γ-Al<sub>2</sub>O<sub>3</sub> catalyst involving the following reactions:



$$\Delta H_{298\text{K}} = -1322 \text{ kJ mol}^{-1}$$



$$\Delta H_{298\text{K}} = -2043 \text{ kJ mol}^{-1}$$

The influence of the reaction products on the oxidation process is discussed and since the oxidation of hydrocarbon mixtures might deviate from the behaviour of the individual hydrocarbons in the absence of other compounds, (see, for example, Spivey [8] and Barresi and Baldi [9]) the influence of ethene on the oxidation of propane has been investigated and vice versa.

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The kinetic experiments were performed in an internal recycle reactor. Such a reactor allows temperature and concentrations gradients to be largely avoided and is therefore very suitable for kinetic experiments.

## 2. Kinetic models

There is no general consensus on the mechanism of catalytic oxidation reactions in the literature (see the review of Spivey [8]). Depending on the specific catalyst and hydrocarbons studied, different mechanisms have been proposed. Under the conditions used in this work, i.e. a large excess of oxygen with propane and ethene as low concentration contaminants and a palladium catalyst, it is usually assumed that chemisorption of oxygen followed by reaction with gaseous hydrocarbon is the mechanism involved. The reaction products, CO<sub>2</sub> and H<sub>2</sub>O, may retard the oxidation reaction. Almost all the authors quoted in the literature have neglected the influence of CO<sub>2</sub>. Assuming that water adsorbs onto the adsorbed oxygen, the following reaction rate expression can be obtained (see Golodets [10] for its detailed derivation):

$$R_{\text{HC}} = \frac{k_2 P_{\text{O}_2} k_1 P_{\text{HC}}}{k_2 P_{\text{O}_2} (1 + K_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}}) + \nu k_1 P_{\text{HC}}} \quad (1)$$

while for the reaction rate constant,  $k_1$ , an Arrhenius temperature dependence is assumed:

$$k_1 = k_{1,\infty} e^{-E_{\text{act}}/RT} \quad (2)$$

Table 1 lists four different rate expressions which have been used to describe the experiments. Models I, II and III can be derived from Eq. (1) with Model III being equivalent to Eq. (1) provided  $k'_1 = \nu k_1 / k_2 P_{\text{O}_2}$ . If the surface reaction is much slower than oxygen adsorption, then  $\nu k_1 P_{\text{HC}} \ll k_2 P_{\text{O}_2}$  and model II is obtained. A further simplification can be achieved by neglecting the influence of water on the process, which is possible if  $K_{\text{H}_2\text{O}} P_{\text{H}_2\text{O}} \ll 1$ : this yields the rate expression given by model I. Model IV is a power law rate expression which cannot be deduced from Eq. (1). Such

Table 1  
Kinetic rate expressions for the complete oxidation of ethene and propane

Model	Reaction rate expression
I	$R_{\text{HC}} = k_{1,\infty} e^{-E_{\text{act}}/RT} \cdot P_{\text{HC}}$
II	$R_{\text{HC}} = \frac{k_{1,\infty} e^{-E_{\text{act}}/RT} \cdot P_{\text{HC}}}{1 + K_{\text{H}_2\text{O}} \cdot P_{\text{H}_2\text{O}}}$
III	$R_{\text{HC}} = \frac{k_{1,\infty} e^{-E_{\text{act}}/RT} \cdot P_{\text{HC}}}{1 + K_{\text{H}_2\text{O}} \cdot P_{\text{H}_2\text{O}} + k'_1 \cdot P_{\text{HC}}}$
IV	$R_{\text{HC}} = k_{r,\infty} e^{-E_{\text{act}}/RT} \cdot P_{\text{HC}}^n \cdot P_{\text{H}_2\text{O}}^m$

a model does not provide any insight into the mechanism of the reaction. However, for engineering purposes, it might be convenient and often yields good results provided it is not used for extrapolation outside the experimental range.

## 3. Experimental details

Figure 1 shows a schematic drawing of the experimental installation. Experiments were performed in a Berty-type internal recycle reactor with a volume of 0.5 l. The reactor basket was filled with 10–30 g of the Pd/Al<sub>2</sub>O<sub>3</sub> catalyst. For details of the catalyst, see Table 2. A magnetically driven impeller provided internal recirculation of the gas in the reactor, the rotational speed of the impeller being controlled by an electronic frequency controller with a maximum speed of ca. 1500 rpm. The catalyst and gas temperatures were measured in the top part of the catalyst bed using two K-type thermocouples. The temperature in the reactor was regulated by means of an eurotherm temperature controller. The reactor pressure was maintained at its set-point by means of a mechanical back-pressure controller. The maximum allowable pressure in the system was 5 bar, as measured at the top of the reactor with a TransInstruments electron pressure gauge.

Air containing small amounts of ethene and/or propane was fed into the reactor, the air flow and concentrations of the hydrocarbons being controlled by means of Brooks thermal mass flow controllers. Water could be added to the feed by leading part of the air stream through a water evaporation vessel, the water concentration being varied by changing the air flow through the vessel. Additional CO<sub>2</sub> could also be introduced to the feed. In case of emergency or when the system needed to be purged, nitrogen was fed into the reactor instead of the usual feed.

The hydrocarbon concentrations in the inlet and outlet streams were measured using a Varian gas chromatograph equipped with a 2 m × 1/8 in column packed with 80–100 mesh Deactigel. The column was operated at 60 °C. A flame ionisation detector was used for detecting the hydrocarbons. The CO<sub>2</sub> concentration was monitored continuously using a Mairhak 610 CO<sub>2</sub> infrared analyzer. Unfortunately, it was not possible to monitor the CO concentration. The water concentration in the inlet stream was determined using a Panametrics chilled-mirror dew point hygrometer.

Since the inlet and outlet concentrations of the hydrocarbons and CO<sub>2</sub> were determined, overall mass balance of the reactor led to the following equation for the experimental reaction rate:

$$R_{\text{exp}} = \frac{F_{i,j} - F_{\text{out},j}}{M_{\text{cat}}} \quad (3)$$

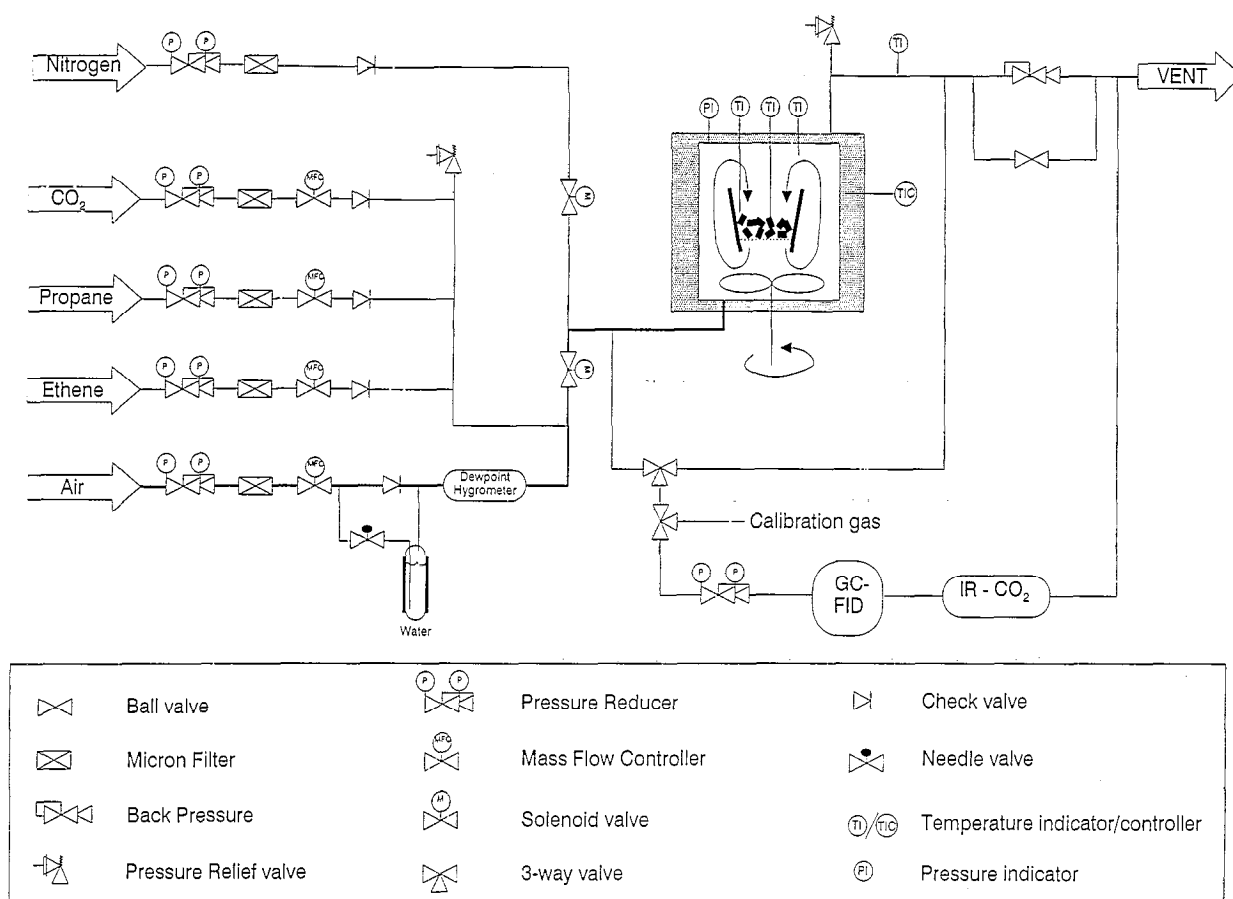


Fig. 1. Schematic drawing of experimental set-up employed.

Estimation of the parameters in the kinetic rate expressions listed in Table 1 was achieved using the SIMUSOLV program of Dow Chemical [11]. This program determines the optimum parameter values using the maximum likelihood principle.

#### 4. Results and discussion

The performance of a Berty reactor is mainly controlled by the recycle ratio. This ratio must be sufficiently high to avoid concentration and temperature gradients in the reactor. Wedel and Villadsen [12] have discussed inaccuracies in the kinetic parameters due to

improper performance, particularly as a result of concentration gradients. Borman [13] has proposed a criterion to take account not only of concentration but also of temperature gradients. Since the experimental determination of the recycle ratio is difficult and inaccurate, some experimental tests have been undertaken to check on the appropriate nature of the reactor. These tests showed that (i) the reaction rates were not influenced by the rotation speed  $N$  of the impeller provided  $N$  was greater than 800 rpm; (ii) interchanging the inlet and outlet of the reactor did not affect the conversion rates; and (iii) the temperature difference between the catalyst and the gas was small, being typically less than 1–2 K. Interchanging the inlet and outlet allowed the number of passes through the catalyst bed to be increased by one. From these three tests we conclude that the recycle ratio was sufficiently high to assume the reactor to be perfectly mixed for our kinetic experiments.

First-order kinetics are often assumed for the complete oxidation of hydrocarbons. In Fig. 2, the reaction rate of propane has been plotted as a function of the partial pressure of propane  $P_{\text{propane}}$  for different temperatures. The increase in the reaction rate with increasing  $P_{\text{propane}}$  is less than proportional. This indicates an inhibition by the reaction products or a reaction order less than unity with respect to propane. The lines

Table 2  
Catalyst properties

Pd/ $\gamma$ -Al <sub>2</sub> O <sub>3</sub> cylinders
diameter, 4.5 mm; height, 4.5 mm
particle density, 1327 kg m <sup>-3</sup>
approximate bed density, 796 kg m <sup>-3</sup>
active metal surface area 350 m <sup>2</sup> kg <sup>-1</sup>
BET surface area 192 m <sup>2</sup> g <sup>-1</sup>
Pd content, 0.07 wt.%
Pd on outer surface only; penetration depth, <0.1 mm

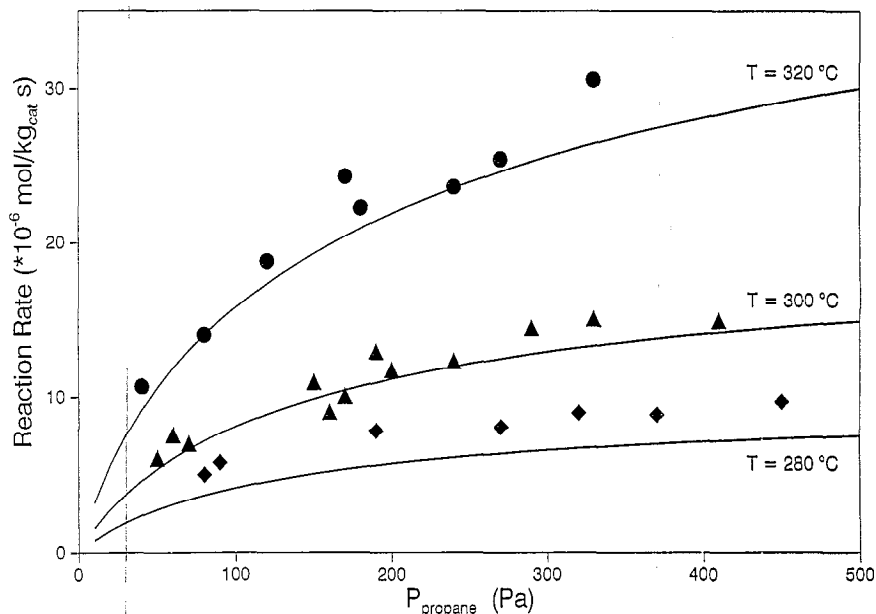


Fig. 2. Reaction rate of propane as a function of the propane partial pressure at different temperatures:  $P = 2.0$  bar, lines calculated using model III (see Tables 1 and 3).

in Fig. 2 were calculated using model III, the most extensive model employed. At low and high temperatures, the model appears to underrate the experimental data but, in general, the agreement is acceptable.

The reaction products,  $\text{CO}_2$  and  $\text{H}_2\text{O}$ , may influence the oxidation of ethene and propane. In most studies quoted in the literature, the influence of  $\text{CO}_2$  was found to be negligible (see, for example, Trimm and Lam [14], Cullis *et al.* [15] and Kemball and Patterson [16]). However, Ribeiro *et al.* [17] observed an abrupt decrease in the methane oxidation rate as soon as the  $\text{CO}_2$

concentration exceeded 0.5 vol.%. Below this value no effect was found. In Fig. 3, the reaction rates of propane and ethene obtained in the present study have been plotted as a function of the  $\text{CO}_2$  concentration, with all other conditions kept constant. The results indicate that neither ethene nor propane oxidation was affected by the addition of  $\text{CO}_2$  to the feed gas.

In contrast to the effect of  $\text{CO}_2$ , most authors have found severe inhibition of the reaction by water. Thus, Ribeiro *et al.* [17] found a reaction order of  $-1$  for  $\text{H}_2\text{O}$  in the oxidation of methane. Simon and Vort-

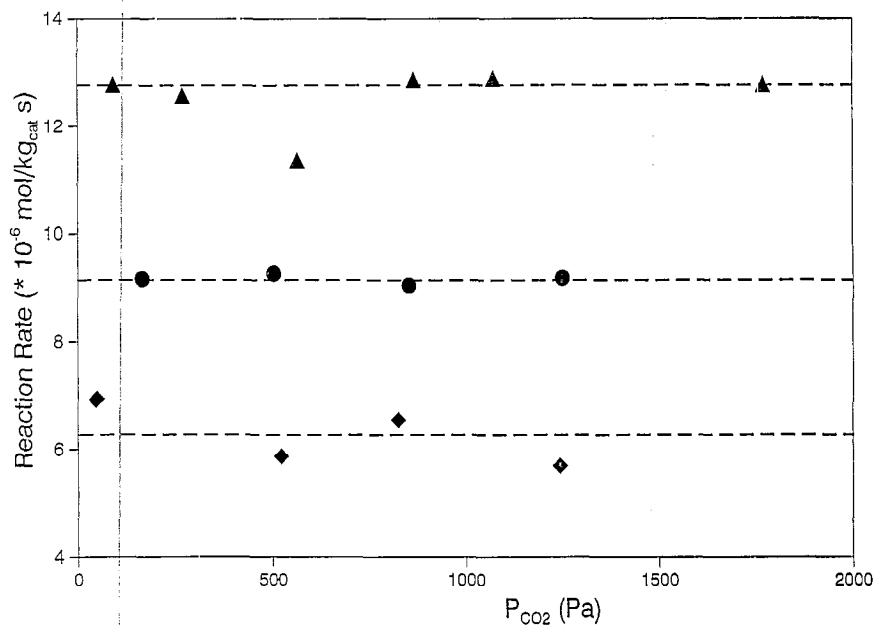


Fig. 3. Influence of  $\text{CO}_2$  on the reaction rates of propane and ethene:  $\blacktriangle$ ,  $P_{\text{ethene}} = 175$  Pa,  $T = 208$  °C;  $\bullet$ ,  $P_{\text{propane}} = 162$  Pa,  $T = 300$  °C;  $\blacklozenge$ ,  $P_{\text{ethene}} = 175$  Pa,  $T = 197$  °C.

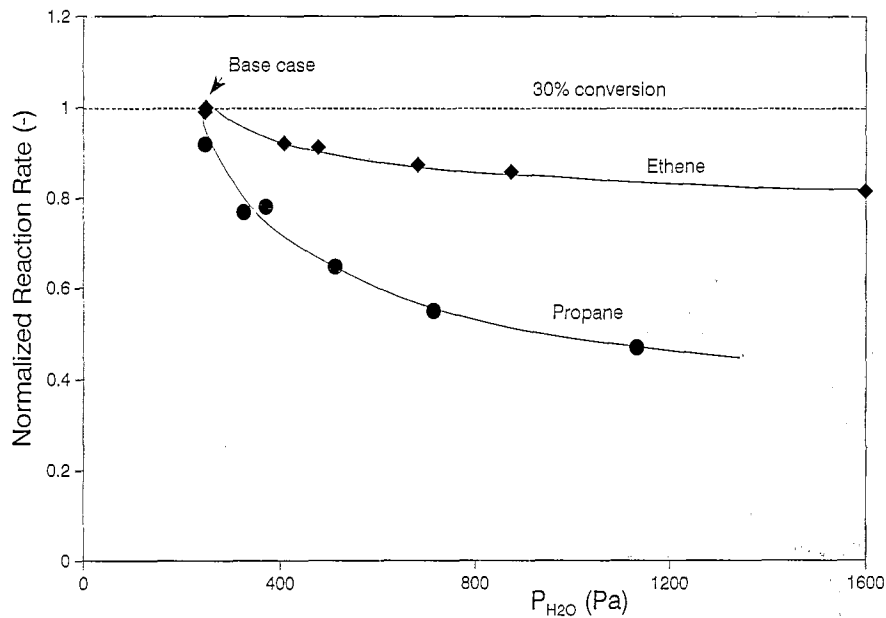


Fig. 4. Influence of water content on the normalized reaction rate of ethene and propane, respectively, defined as the actual reaction rate divided by the reaction rate in the absence of water:  $P = 2$  bar;  $\blacklozenge$ ,  $P_{\text{ethene}} = 250$  Pa,  $T = 208$  °C;  $\bullet$ ,  $P_{\text{propane}} = 182$  Pa,  $T = 300$  °C.

meyer [18] in a study of ethane oxidation on a Pd catalyst found a reaction order for water varying from 0 to  $-0.7$  depending on the temperature employed. However, Kemball and Patterson [16] did not observe any inhibition by water of the oxidation of ethene on Pd. It should be noted that, in contrast to other studies, they used an unsupported catalyst. In Fig. 4, the normalized reaction rate, i.e. the actual reaction rate divided by the rate observed without addition of water or ethene to the feed, has been plotted as a function of the water pressure in the reactor. The results show that

both ethene and propane oxidation are inhibited by water, but the effect on the propane reaction is much stronger with the conversion rate for propane being reduced by a factor of two for high water contents. Using the power law rate expression, the reaction order of water was found to be  $-0.12$  and  $-0.46$  for ethene and propane, respectively.

Mutual inhibition effects were observed during the simultaneous oxidation of ethene and propane. For this reason, we have studied the influence of ethene on propane combustion and vice versa. First we discuss

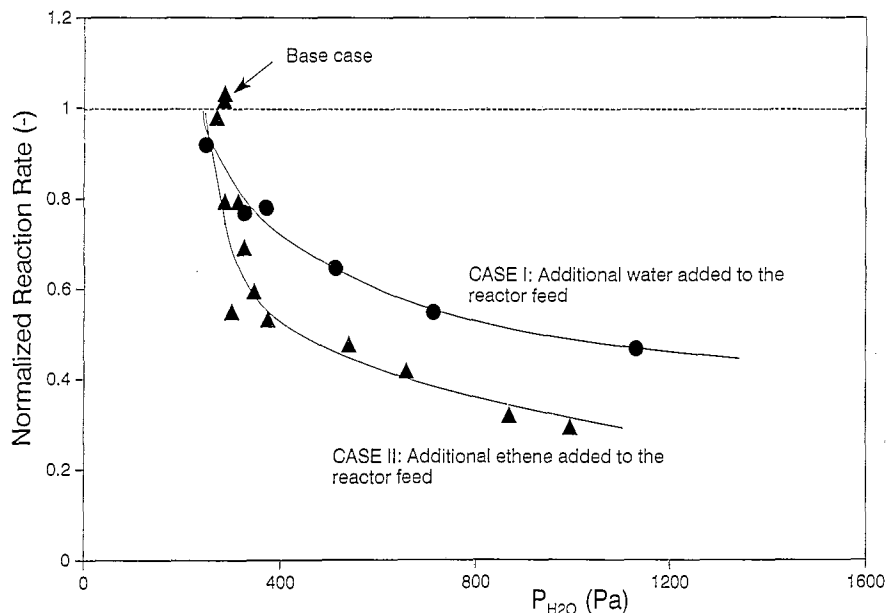


Fig. 5. Influence of water content on the normalized reaction rate for the simultaneous oxidation of ethene and propane, defined as the actual reaction rate divided by the reaction rate in the absence of water or ethene:  $P = 2$  bar;  $\bullet$ ,  $P_{\text{propane}} = 182$  Pa,  $T = 300$  °C;  $\blacktriangle$ ,  $P_{\text{propane}} (= 185 \text{ Pa}) + P_{\text{ethene}} (= 0.250 \text{ Pa})$ ,  $T = 300$  °C.

the influence of ethene on propane oxidation. Under the kinetic conditions employed for the propane reaction, ethene has already reached a very high conversion and hence more H<sub>2</sub>O and CO<sub>2</sub> will be generated. Thus, in comparison to experiments without ethene addition, the H<sub>2</sub>O and CO<sub>2</sub> concentrations in the reactor are higher. Since, as discussed above, water significantly retards propane oxidation, it is possible that the inhibition induced by ethene may also be caused by the increased water concentration. This is supported by the results depicted in Fig. 5, in which the normalized reaction rate of propane combustion is plotted versus the water concentration for two different cases: (i) where the water concentration in the reactor was increased by the addition of water to the reactor feed and (ii) where the water concentration in the reactor was increased by the addition of ethene to the feed and attributed to the consecutive oxidation of ethene to H<sub>2</sub>O and CO<sub>2</sub> in the reactor.

For the base case, i.e. without addition of water or ethene to the feed, the water content in the reactor was about 250 Pa due to the conversion of propane. Figure 5 shows that in both instances the reaction rate for propane oxidation decreased with increasing water concentration. Conversions were between 70% and 90% for ethene and between 15% and 30% for propane, respectively. In addition the decrease in the oxidation rate for propane was larger for case II than for case I. In case II, only ethene was added and hence the decrease in activity was caused by the water produced and by another inhibiting agent. It is assumed that the presence of unconverted ethene or of an (unknown) adsorbed intermediate product also retards the oxidation of propane, since CO<sub>2</sub> was shown to have no effect.

The addition of propane did not affect the reaction of ethene. In these experiments, the temperature employed was so low that the conversion of propane was negligible.

The models listed in Table 1 have been fitted to the experimental data. Best fit values for the kinetic parameters of these models are listed in Table 3. Fig-

ures 6 and 7 show a comparison of the measured reaction rates with the model predictions for ethene and propane, respectively. In both cases model I, i.e. the simplest model, gives the poorest results. However, for the combustion of ethene, model II, III and IV perform equally well. For the oxidation of propane, the best results are obtained with model IV. Despite the slightly higher mean error involved, model III is preferred for the prediction of the reaction rate of propane because its derivation is based on a reaction mechanism.

We also used a different experimental installation to obtain numerical values for the kinetic parameters. For a detailed description, refer to van de Beld *et al.* [7]. The main differences were:

1. A dynamic method (DM) was used. The reactor was operated under transient conditions whereas the Berty reactor was operated in a stationary state. The dynamic method was much faster, but less accurate.
2. The reactor behaved like a plug-flow reactor whereas the Berty reactor should be perfectly mixed.

The kinetic data obtained from both installations could be compared by calculating the conversion versus temperature profiles for an isothermal plug-flow reactor, for which the following mass balance applies:

$$0 = - \frac{d(u_g C_j)}{dz} - R_j(1 - \epsilon)\rho_s \quad (4)$$

The reaction rate  $R_j$  may be calculated using the models and data given in Tables 1 and 3, respectively. The rate expression for the dynamic method is similar to model I. The curves for total conversion versus temperature were calculated as follows: at a given operating temperature, the total conversion over the reactor may be calculated by integrating Eq. (4) for an isothermal reactor with a certain bed length. This led to an outlet conversion for the chosen kinetic model and reactor temperature. The process was then repeated for the various models and temperatures.

Figure 8 shows plots of the calculated conversion for ethene and propane derived from the different kinetic

Table 3

Best fit values for parameters involved in the oxidation of ethene and propane as derived from the various models listed in Table 1

Parameter	Ethene					Propane				
	DM <sup>a</sup>	I	II	III	IV	DM <sup>a</sup>	I	II	III	IV
$E_{act}$ (kJ mol <sup>-1</sup> )	67.3	57.8	58.9	57.4	43.2	87.7	92.9	153.7	101.2	119.3
$k_{1,\infty}$ or $k_{r,\infty}$	$1.2 \times 10^0$	$1.8 \times 10^{-1}$	$3.2 \times 10^{-1}$	$2.3 \times 10^{-1}$	$4.3 \times 10^2$	$7.2 \times 10^0$	$1.4 \times 10^1$	$9.9 \times 10^8$	$3.2 \times 10^2$	$4.8 \times 10^5$
$K_{H_2O}$ (Pa <sup>-1</sup> )	–	–	$9.4 \times 10^{-4}$	$8.7 \times 10^{-4}$	–	–	–	$5.3 \times 10^{-1}$	$1.5 \times 10^{-3}$	–
$k'_1$ (Pa <sup>-1</sup> )	–	–	–	$2.3 \times 10^{-4}$	–	–	–	–	$9.1 \times 10^{-3}$	–
$n$	–	–	–	–	0.71	–	–	–	–	0.61
$m$	–	–	–	–	-0.12	–	–	–	–	-0.46
Error (%)	–	19.7	16.6	16.4	16.6	–	31.8	17.6	13.7	12.5

<sup>a</sup>Data obtained from experiments using a dynamic method. Reaction rate expression same as in model I (see Ref. [7]).

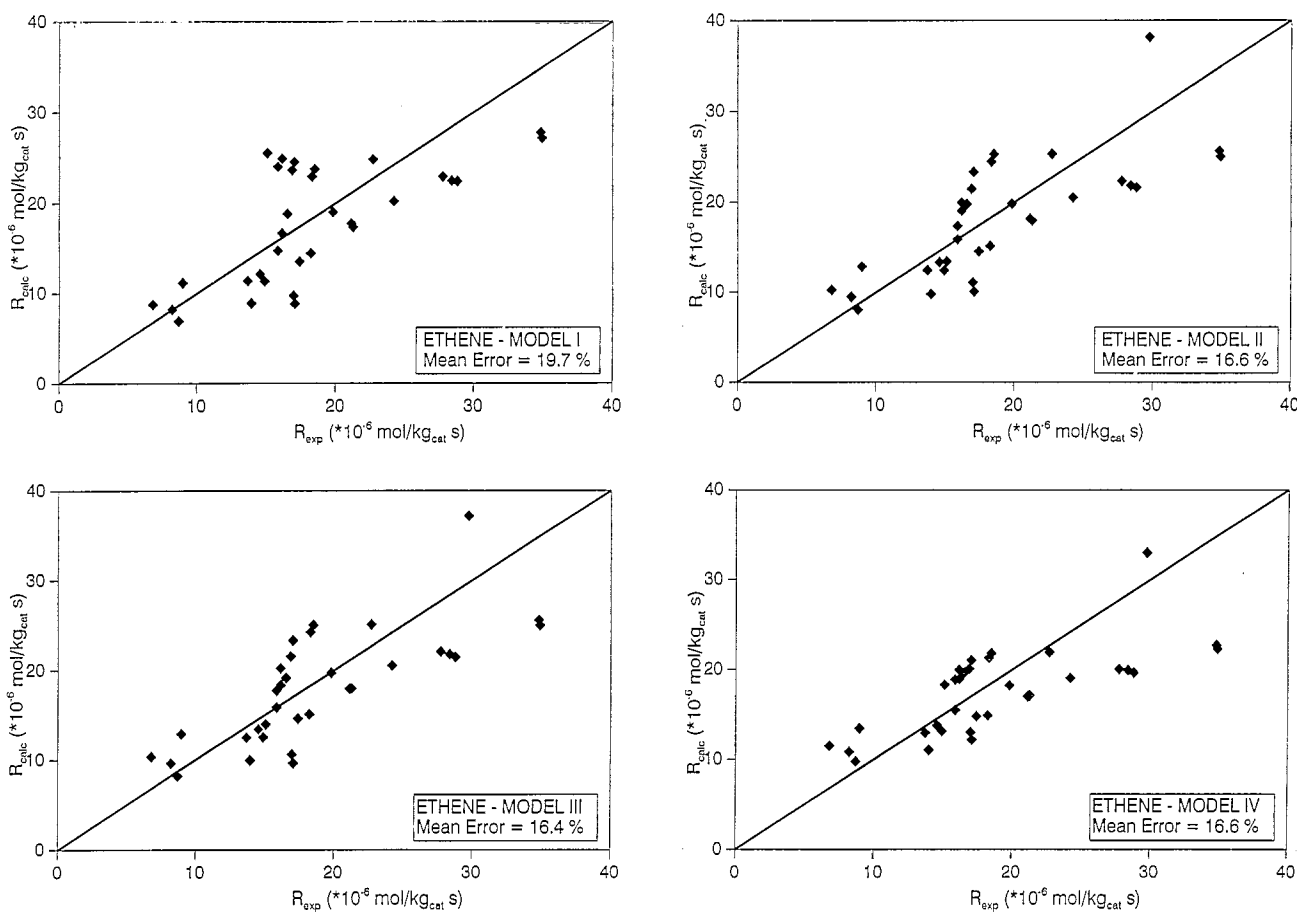


Fig. 6. Calculated reaction rates for ethene oxidation according to the different models versus the measured values. For models employed, see Table 1

models as a function of the bed temperature in the reactor. Under the usual operating conditions applied, the calculated conversions for kinetic models I–IV are comparable. Extrapolation to higher temperatures led to significant differences for both components.

The conversion profile has also been calculated by making use of the kinetic data obtained with the dynamic method DM. This profile is compared to the results obtained with model III in Fig. 9. Although the agreement is satisfactory for the oxidation of propane, significant differences are observed for the oxidation of ethene. Thus, when the kinetic data obtained with the dynamic method DM are employed, a higher conversion of ethene is found. Hence the activity of the catalyst used in the Berty reactor appears to be lower. This apparent difference in activity may be explained by the different conditions under which the catalyst is exposed in both installations, with a constant catalyst activity being difficult to achieve in the Berty reactor.

Over a substantial period of time, the rate of ethene oxidation decreased with time on-stream. However, the original activity could be regained by treatment of the catalyst at higher temperatures. This is illustrated in Fig. 10 where the catalyst was first exposed to ethene oxidation for 2 h at 320 °C. The experiment was then

repeated, and it was observed that initially ethene conversion was even higher than previously. Similar observations have been made by Hawkins and Wanke [19] for ethene oxidation over a Pt catalyst. Such reversible catalyst deactivation did not occur with the dynamic method since in that case the catalyst was heated up to 600 °C prior to carrying out the oxidation reaction. Hence, with the dynamic method, the catalyst always operated at high initial activity and for this reason, depending on the operating conditions, the kinetic data obtained with the dynamic method probably give a more correct prediction of the behaviour of a catalytic packed-bed reactor, despite the lower accuracy of this method.

## 5. Conclusions

Kinetic experiments for the total oxidation of ethene and propane, and of their mixtures on a Pd/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst have been carried out in a Berty reactor. The influence of the reaction products, H<sub>2</sub>O and CO<sub>2</sub>, was also investigated. The addition of CO<sub>2</sub> to the feed did not alter the rates of oxidation. However, water strongly retarded the conversion rates for both ethene

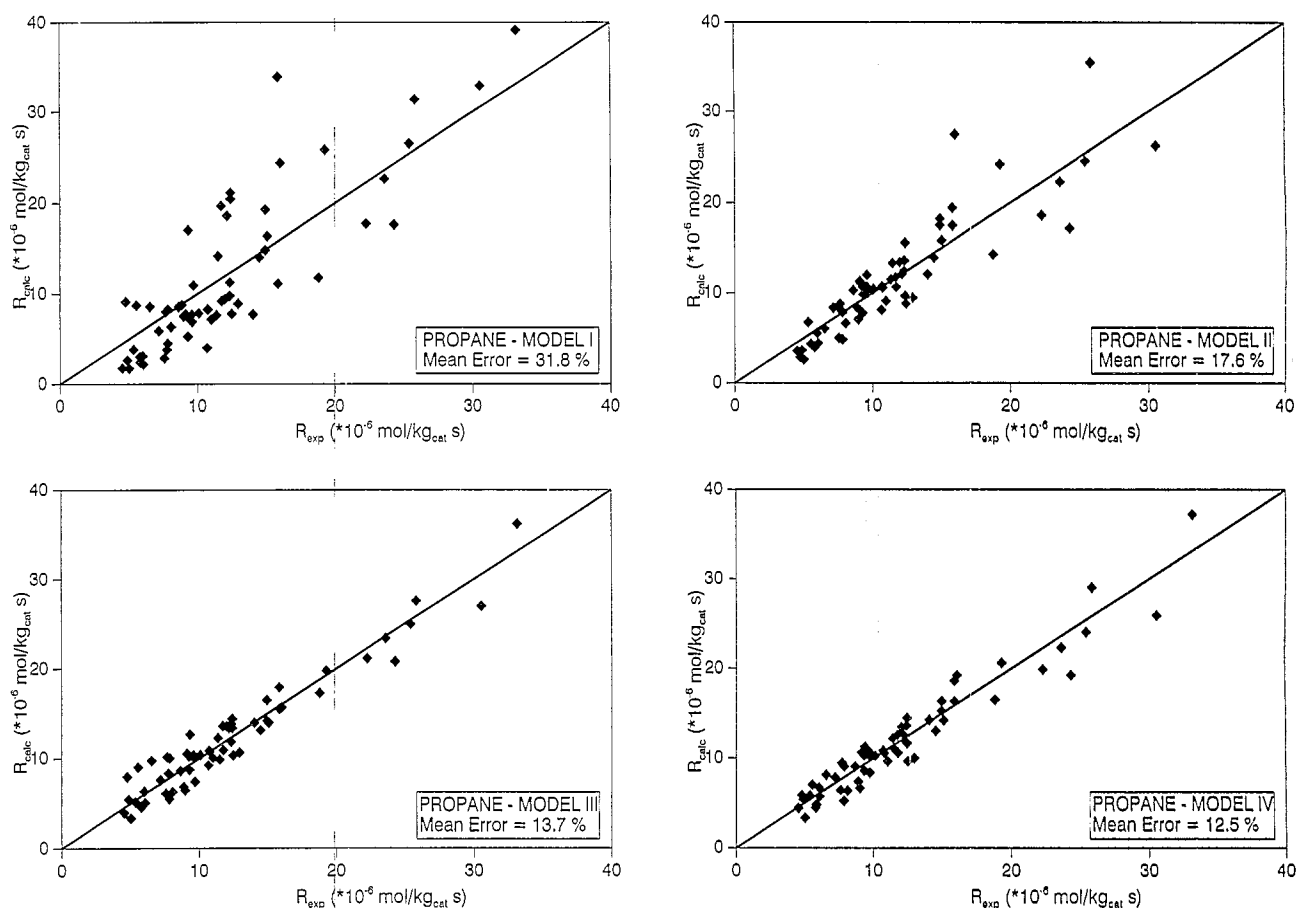


Fig. 7. Calculated reaction rates for propane oxidation according to the different models versus the measured values. For models employed, see Table 1.

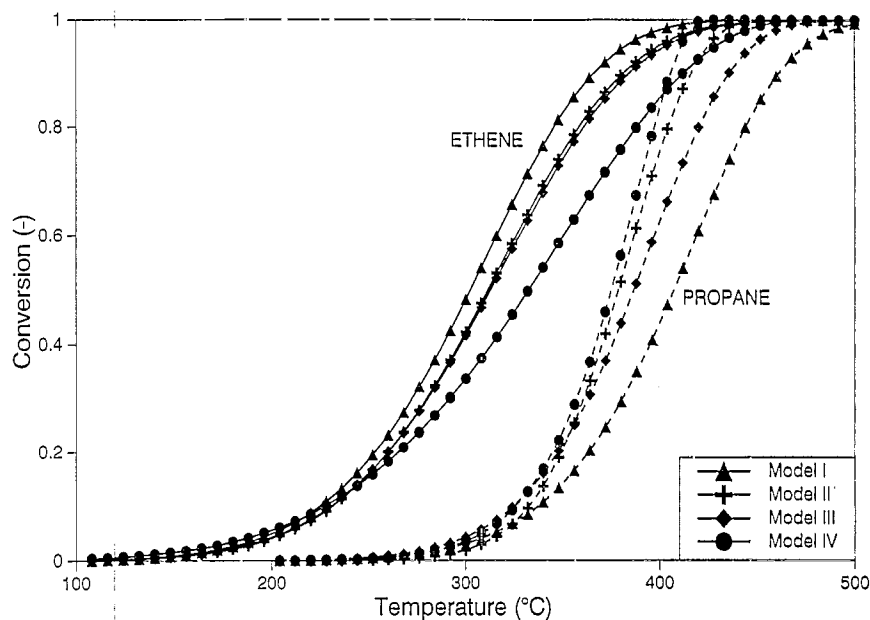


Fig. 8. Calculated conversions for the individual oxidations of ethene and propane as a function of the operating temperature for an isothermal packed-bed reactor using the different kinetic models listed in Table 1. The kinetic data used in the calculations are given in Table 3. The following values were employed:  $u_g = 0.20 \text{ m s}^{-1}$ ,  $L = 0.10 \text{ m}$ ,  $C_{\text{propane, in}} = 1000 \text{ ppm}$ ,  $C_{\text{ethene, in}} = 1000 \text{ ppm}$ .

and propane. Through the use of a power law rate expression, the reaction order of water was determined as  $-0.12$  and  $-0.46$  for ethene and propane, respec-

tively. The rate of oxidation for propane decreased when ethene was present in the feed. Under the conditions employed for propane oxidation, ethene conver-



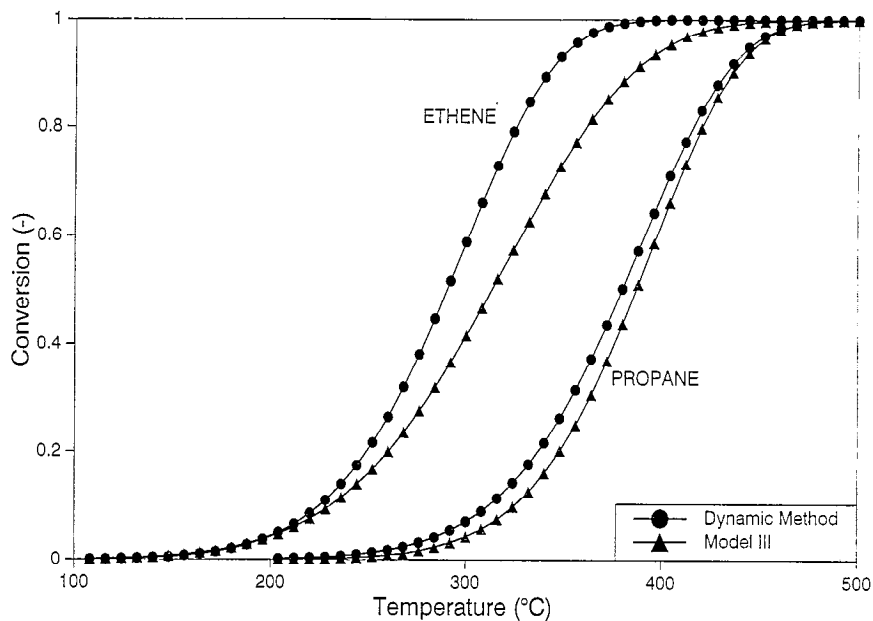


Fig. 9. Calculated conversions for the individual oxidations of ethene and propane as a function of the operating temperature for an isothermal packed-bed reactor. The kinetic data used in the calculations are given in Table 3. The following values were employed:  $u_g = 0.20 \text{ m s}^{-1}$ ,  $L = 0.10 \text{ m}$ ,  $C_{\text{ethene, in}} = 1000 \text{ ppm}$ ,  $C_{\text{propane, in}} = 1000 \text{ ppm}$ .

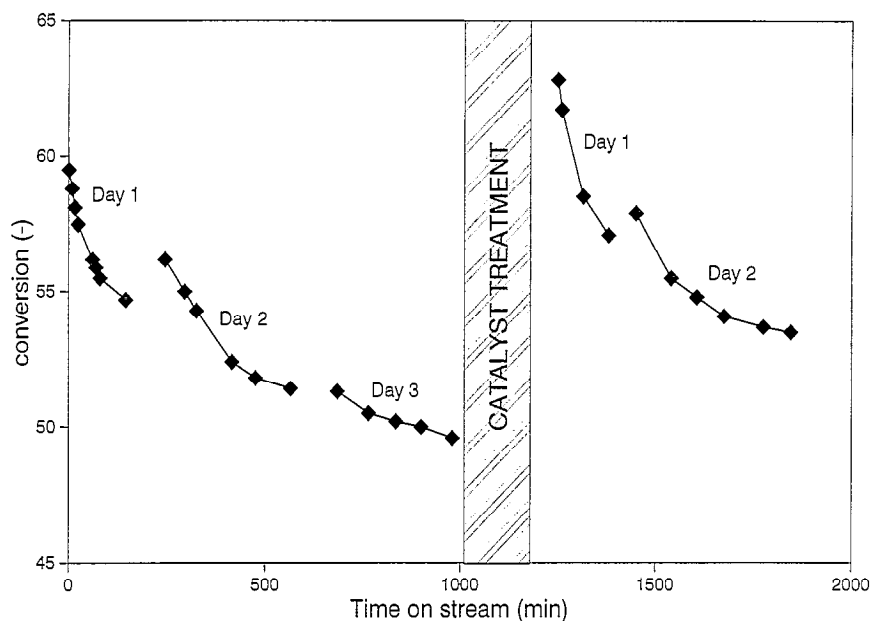


Fig. 10. Ethene conversion as a function of time on-stream:  $P = 2.00 \text{ bar}$ ,  $T = 220 \text{ }^\circ\text{C}$ ,  $C_{\text{ethene, in}} = 2630 \text{ ppm}$ ; catalyst treatment,  $T = 320 \text{ }^\circ\text{C}$ . All other conditions remained the same.

sion is already high and significant amounts of water were produced. However, the additional water formed by the conversion of ethene did not completely explain such inhibition by ethene. In the studies undertaken, the conversions were between 70% and 90% for ethene, and between 15% and 30% for propane. Ethene oxidation was not affected by the presence of propane.

Four different reaction rate expressions have been tested for fitting the experimental data. The best rate expressions fitted the experimental data with an average

error of 17% for ethene oxidation and 13% for propane oxidation, respectively.

On the basis of conversion profiles calculated for a packed-bed reactor, the kinetic data were compared with results obtained using a dynamic measuring technique. Good agreement was observed for propane oxidation. However, with ethene combustion the conversion rate calculated using the kinetic data from the Bertly reactor was lower which may be explained by differences in the operating conditions for both reactors.

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## Nomenclature

$C$	concentration, $\text{mol m}^{-3}$
$E_{\text{act}}$	activation energy, $\text{J mol}^{-1}$
$F$	molar flow rate, $\text{mol s}^{-1}$
$k_1$	reaction rate constant, $\text{mol kg}^{-1} \text{s}^{-1} \text{Pa}^{-1}$
$k_{1,\infty}$	pre-exponential factor, $\text{mol kg}^{-1} \text{s}^{-1} \text{Pa}^{-1}$
$k_2$	rate constant of oxygen adsorption, $\text{mol kg}^{-1} \text{s}^{-1} \text{Pa}^{-1}$
$k_r$	reaction rate constant, $\text{mol kg}^{-1} \text{s}^{-1} \text{Pa}^{n+m}$
$k_{1,\infty}$	$= k_1/k_2 P_{\text{O}_2}$ , $\text{Pa}^{-1}$
$k_{r,\infty}$	pre-exponential factor, $\text{mol kg}^{-1} \text{s}^{-1} \text{Pa}^{n+m}$
$K$	adsorption constant, $\text{Pa}^{-1}$
$M_{\text{cat}}$	catalyst mass, $\text{kg}$
$N$	rotation speed of the impeller, $\text{s}^{-1}$
$P$	(partial) pressure, $\text{Pa}$
$R$	gas constant, $\text{J mol}^{-1} \text{K}^{-1}$
$R_{\text{HC}}$	reaction rate, $\text{mol HC converted kg}_{\text{cat}}^{-1} \text{s}^{-1}$
$R_{\text{exp}}$	experimentally determined reaction rate, $\text{mol HC converted kg}_{\text{cat}}^{-1} \text{s}^{-1}$
$T$	temperature, $\text{K}$
$u_g$	superficial gas velocity, $\text{m s}^{-1}$
$x$	mole fraction, –
$z$	axial position, $\text{m}$
$\varepsilon$	bed porosity, –
$\rho_s$	density of the catalyst, $\text{kg m}^{-3}$
$\nu$	stoichiometric coefficient, –

## Subscripts and superscripts

f	feed
HC	hydrocarbon
$j$	component $j$
$m$	reaction order with respect to water, see model IV
$n$	reaction order with respect to hydrocarbon, see model IV
out	outlet

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