Mechanism of the catalytic soot oxidation on Fe_2O_3

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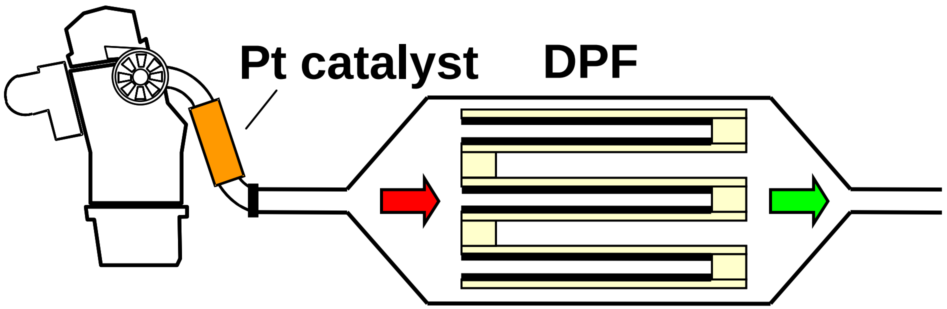
Removal of soot from diesel exhaust

- **Separation of soot by Diesel Particulate Filters (DPF)**



- **DPF regeneration**
  - Continuously Regeneration Trap (CRT)

$$NO + 0{,}5\ O_2 \xrightarrow{Pt} NO_2$$

$$„C“ + 2\ NO_2 \longrightarrow 2\ NO + CO_2$$

  - Catalytic DPF (C-DPF)

$$„C“ + O_2 \longrightarrow CO_2$$ Catalysts: CeO_2, Fe_2O_3

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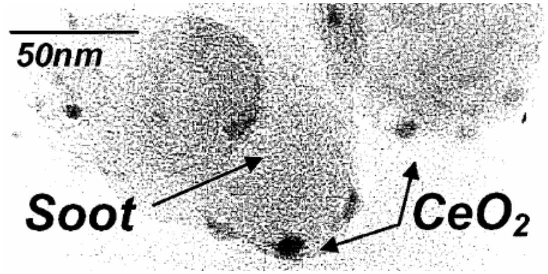
- CeO_2 and Fe_2O_3 originated from Fuel Borne Catalysts (FBC) enhance oxidation of deposited soot



K. Ohno, Ph.D. thesis, 2006

➡ **Fe_2O_3 reveals practical relevance for catalytic soot oxidation**

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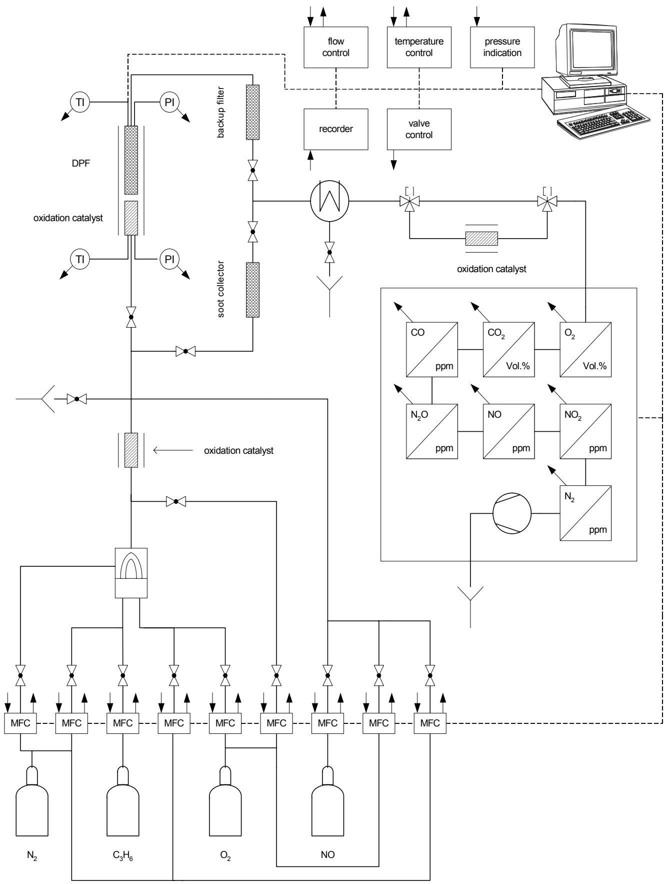
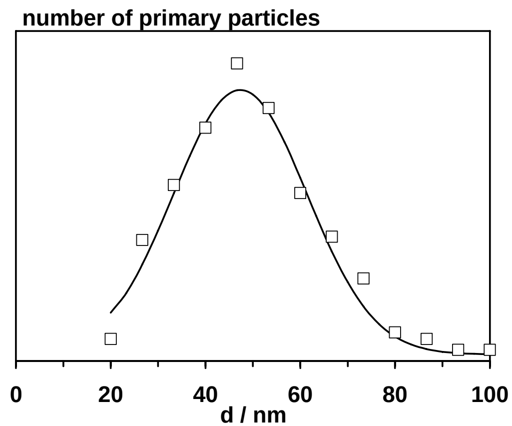
- In our mechanistic studies: α-Fe_2O_3 and a C_3H_6 soot are used
- Model soot prepared by diffusion burner (C_3H_6/O_2 flame)



- 2.6 wt.% adsorbed species
- 98.8 wt.% C
  0.7 wt.% O
  0.5 wt.% H
  0 wt.% N
- S_{BET} = 65 m²/g
- d = 45 nm (most frequent diameter)



P. Balle, H. Bockhorn, B. Geiger, N. Jan, S. Kureti, D. Reichert, T. Schröder, *Chem. Eng. Process.* 45 (2006) 1065

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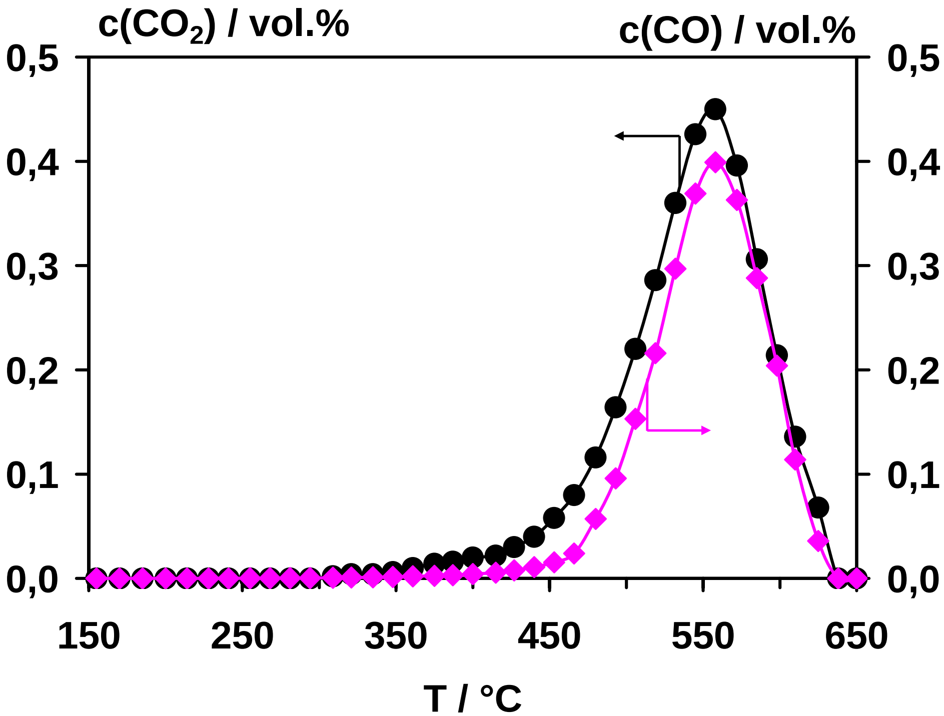
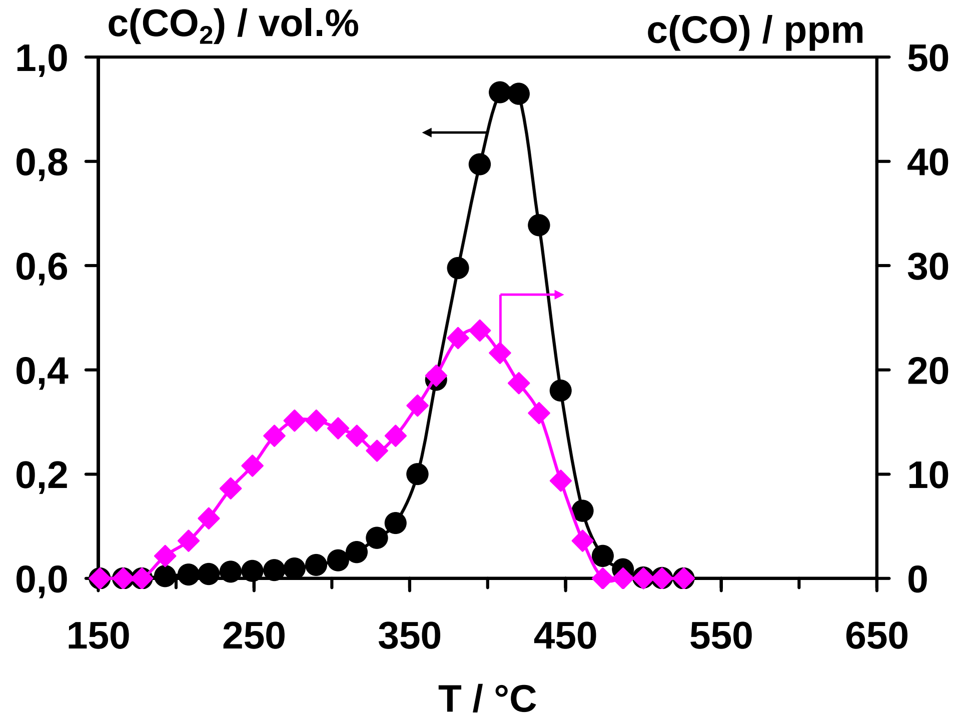
Effect of the Fe_2O_3 catalyst in Temperature Programmed Oxidation (TPO) of the soot

without catalyst



with Fe_2O_3 catalyst



Conditions: $c(O_2)$=6.0 vol.% Flow: 500 ml/min (STP) $\Delta T/\Delta t$=90 K/h
$c(N_2)$=94 vol.% $n(Fe_2O_3)$=20 mmol n(C)=10 mmol

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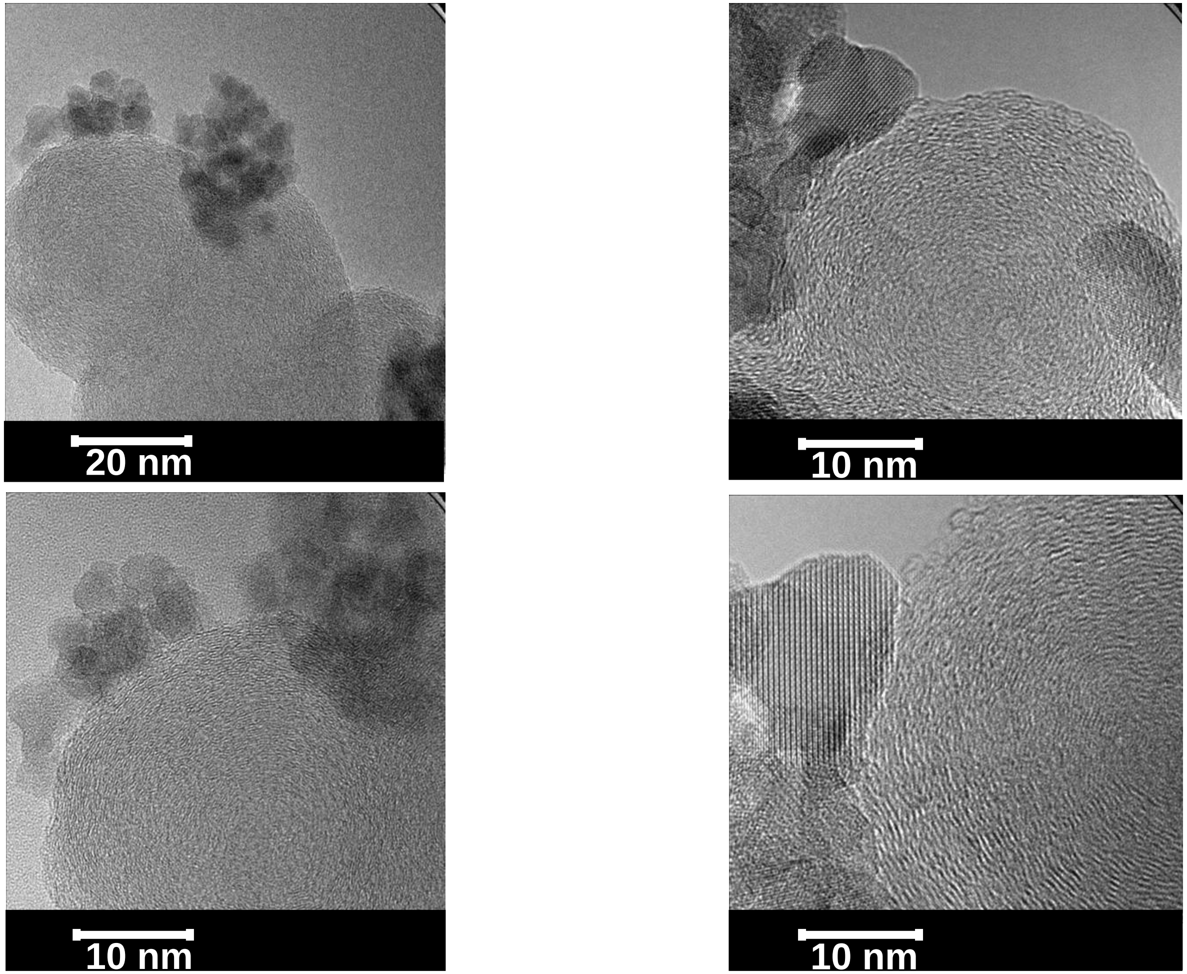
Development of the contact between Fe_2O_3 catalyst and soot (HRTEM study)



X(soot) = 0% | **X(soot) = 90%**

H. Bockhorn, S. Kureti, D. Reichert, *Top. Catal.* (2007)

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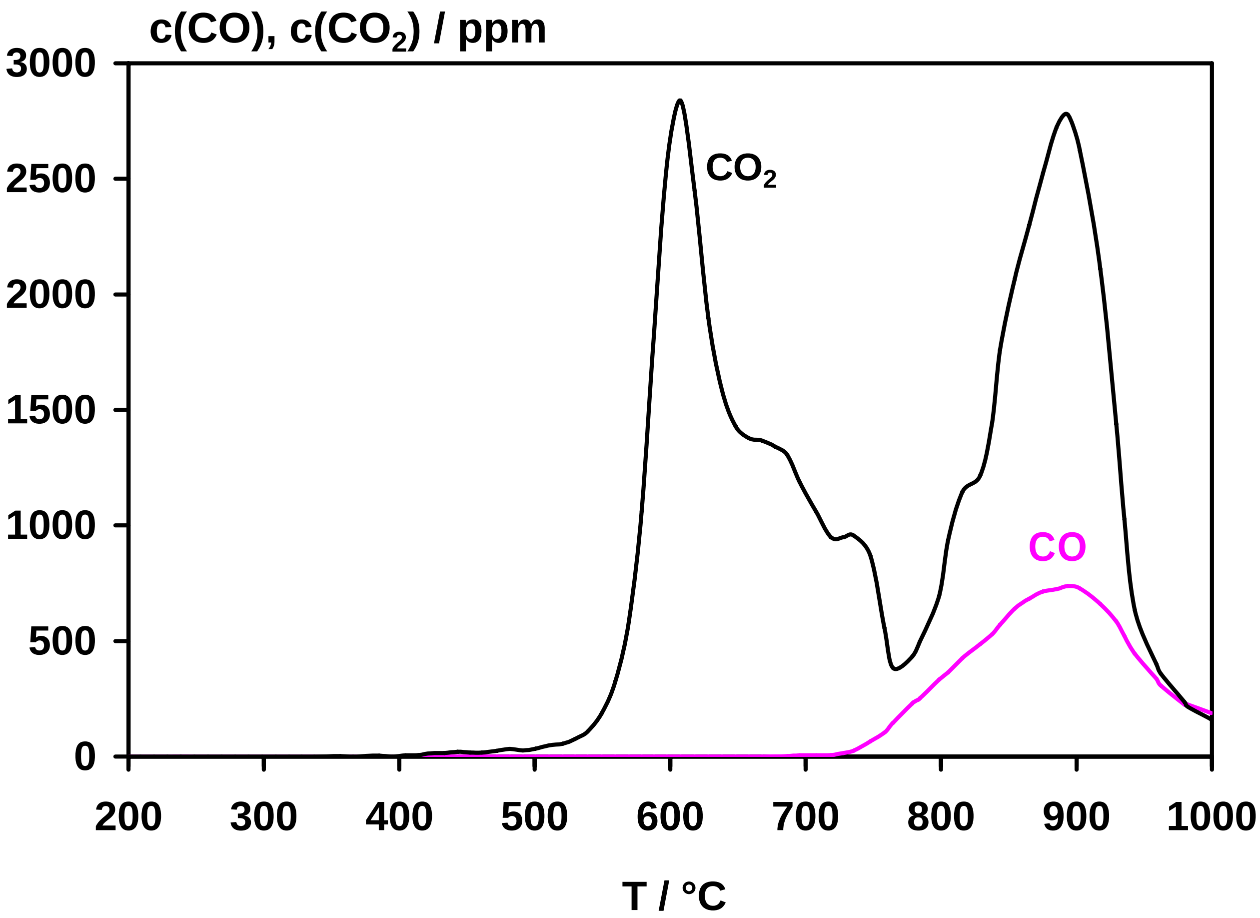
Carbothermal reaction



Conditions:

$c(O_2)$=0 vol.%

N_2 balance

$n(Fe_2O_3)$=20 mmol

n(C)=10 mmol

$\Delta T/\Delta t$=90 K/h

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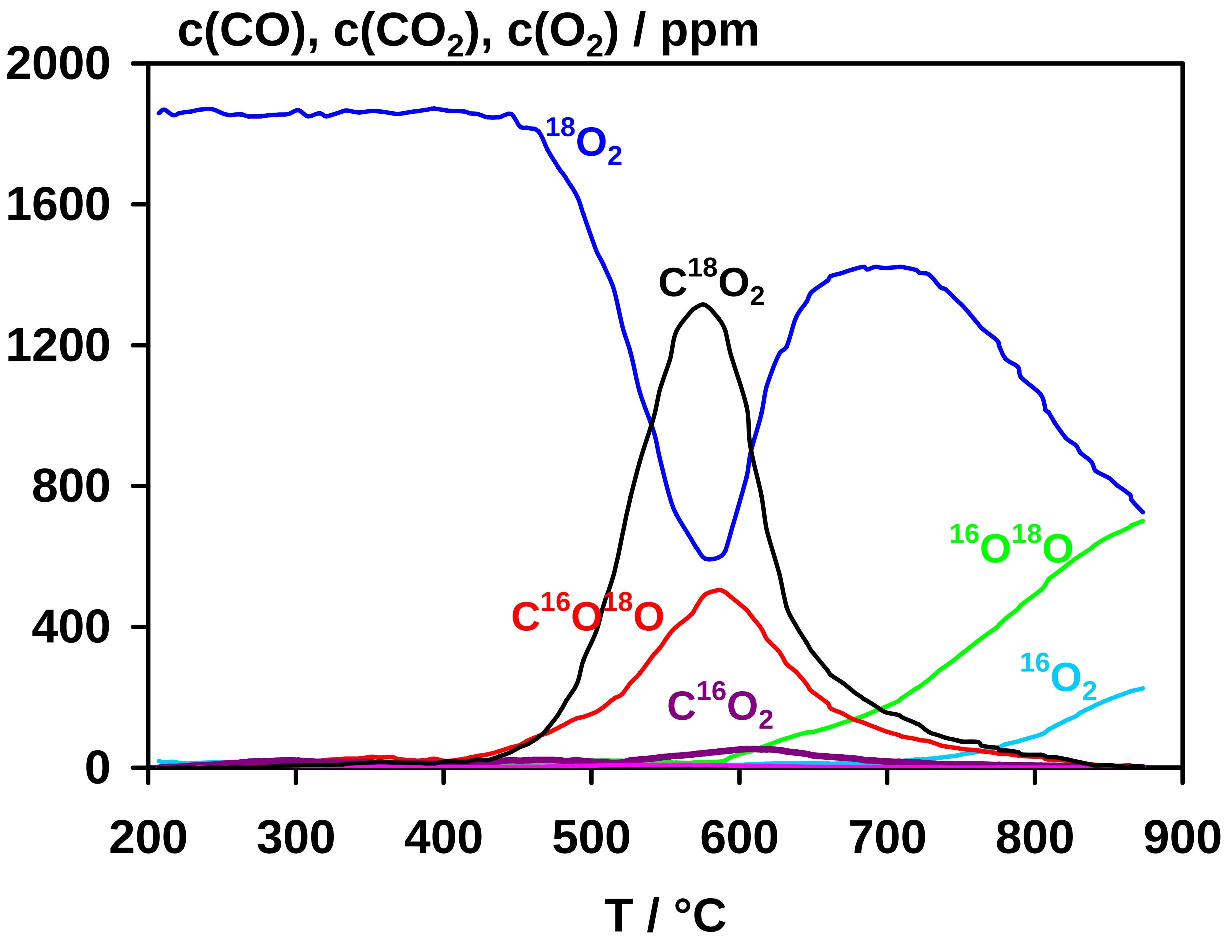
TPO with isotope labelled oxygen ($^{18}O_2$)



Conditions:

$c(O_2)$=0.19 vol.%

N_2 balance

$n(Fe_2O_3)$=3.8 mmol

n(C)=1.9 mmol

$\Delta T/\Delta t$=600 K/h

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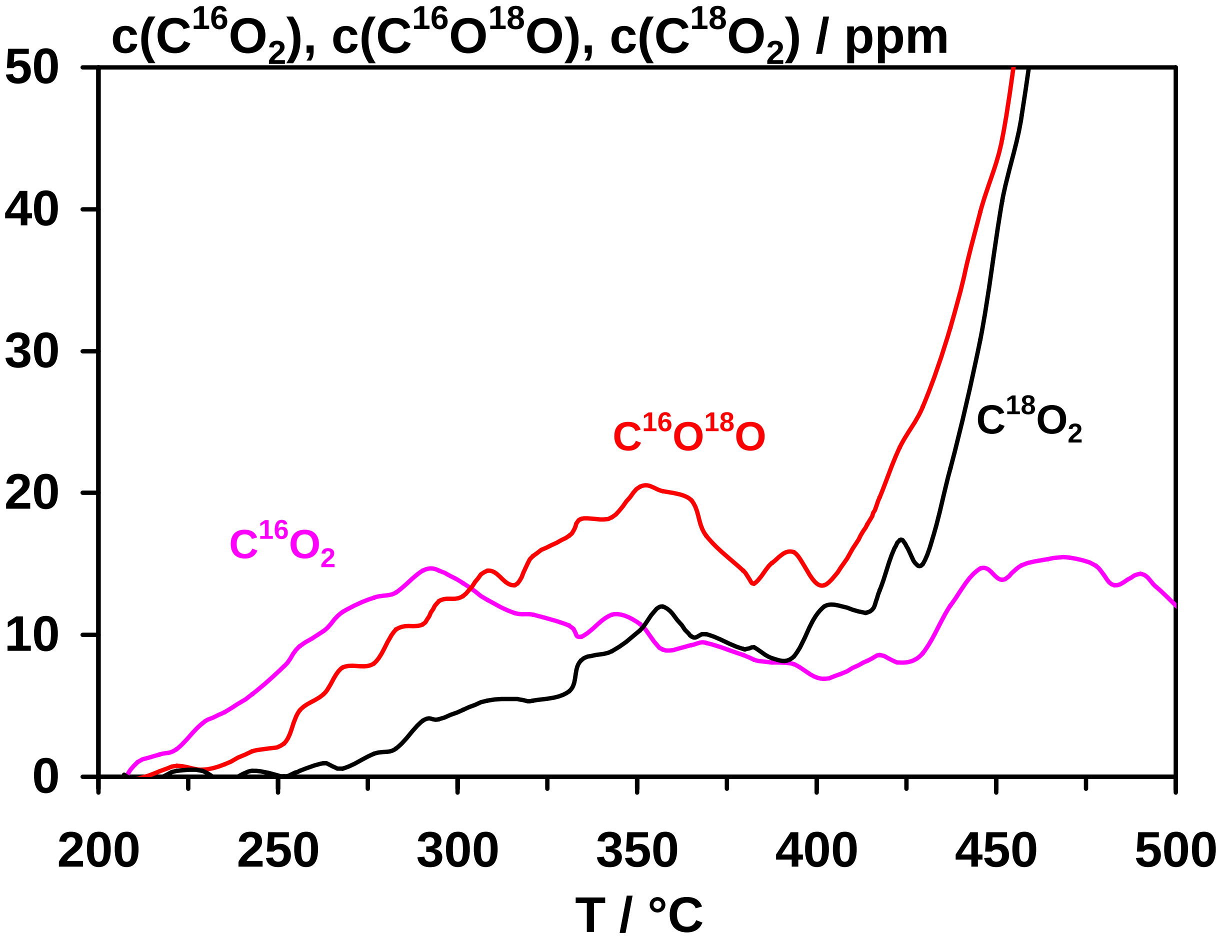
Starting period of the isotopic TPO



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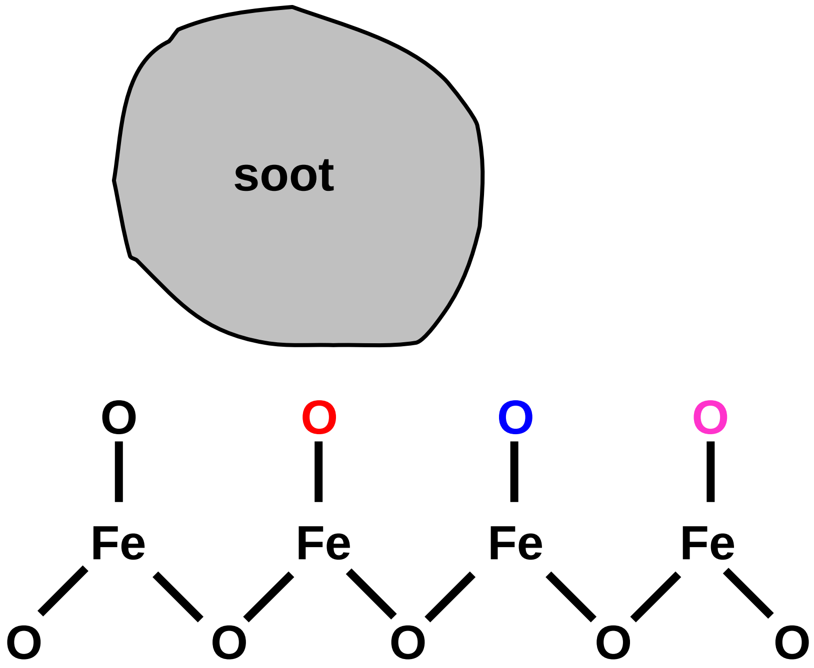
Model for the effect of Fe_2O_3 catalyst on soot oxidation



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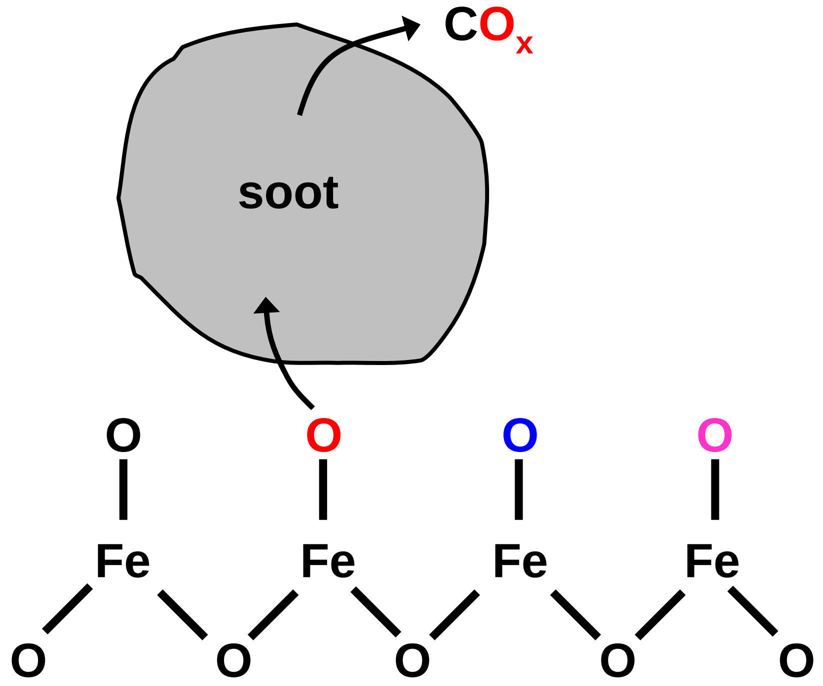

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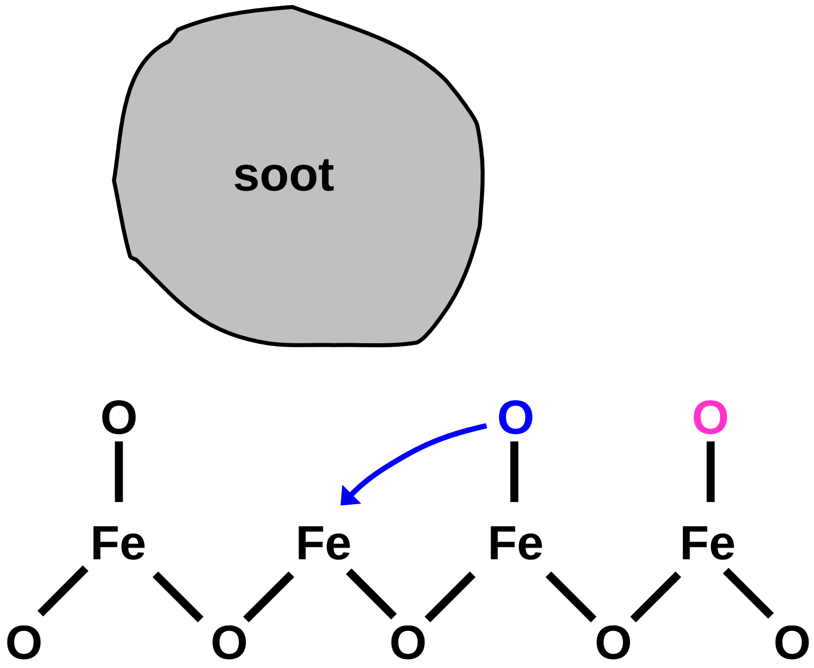

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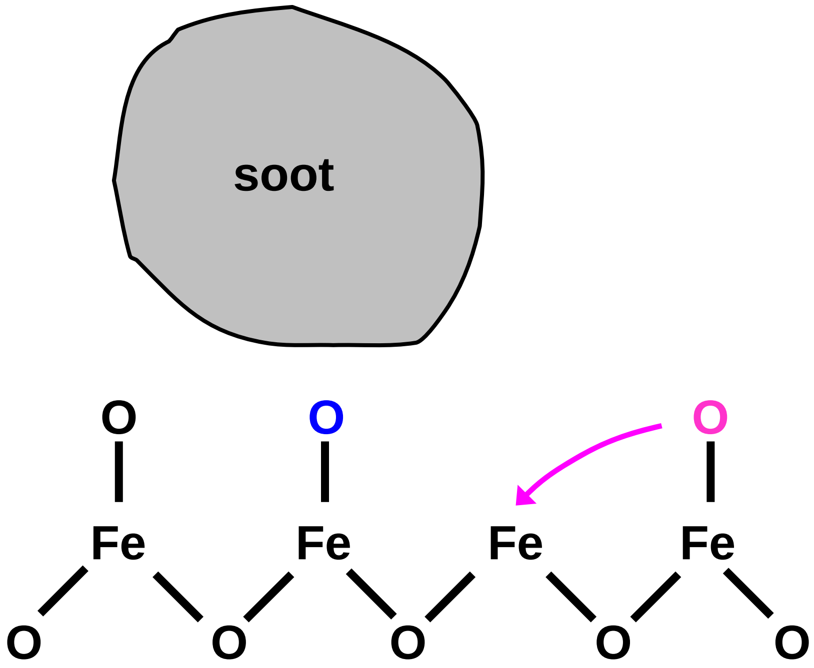

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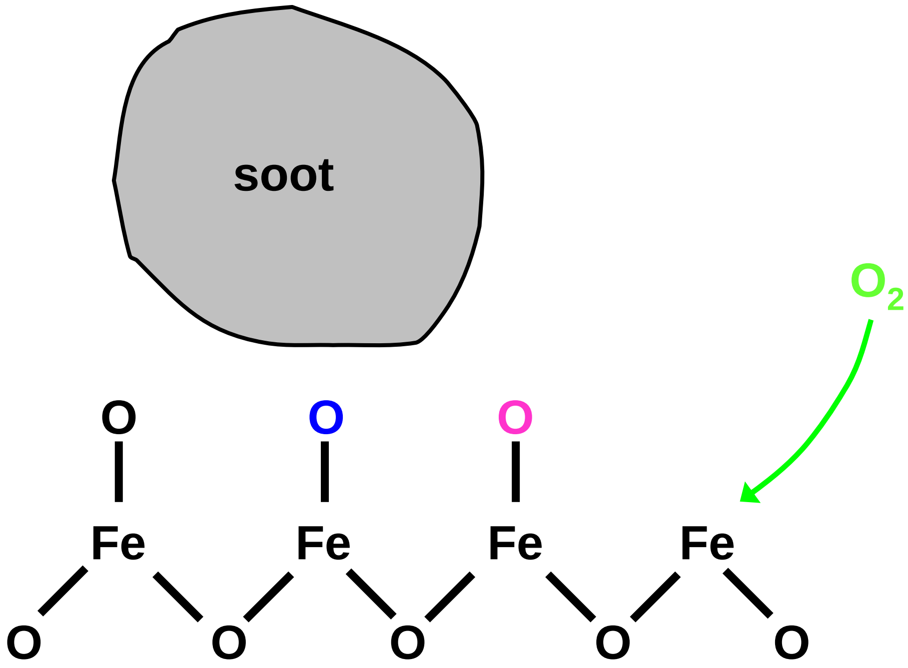

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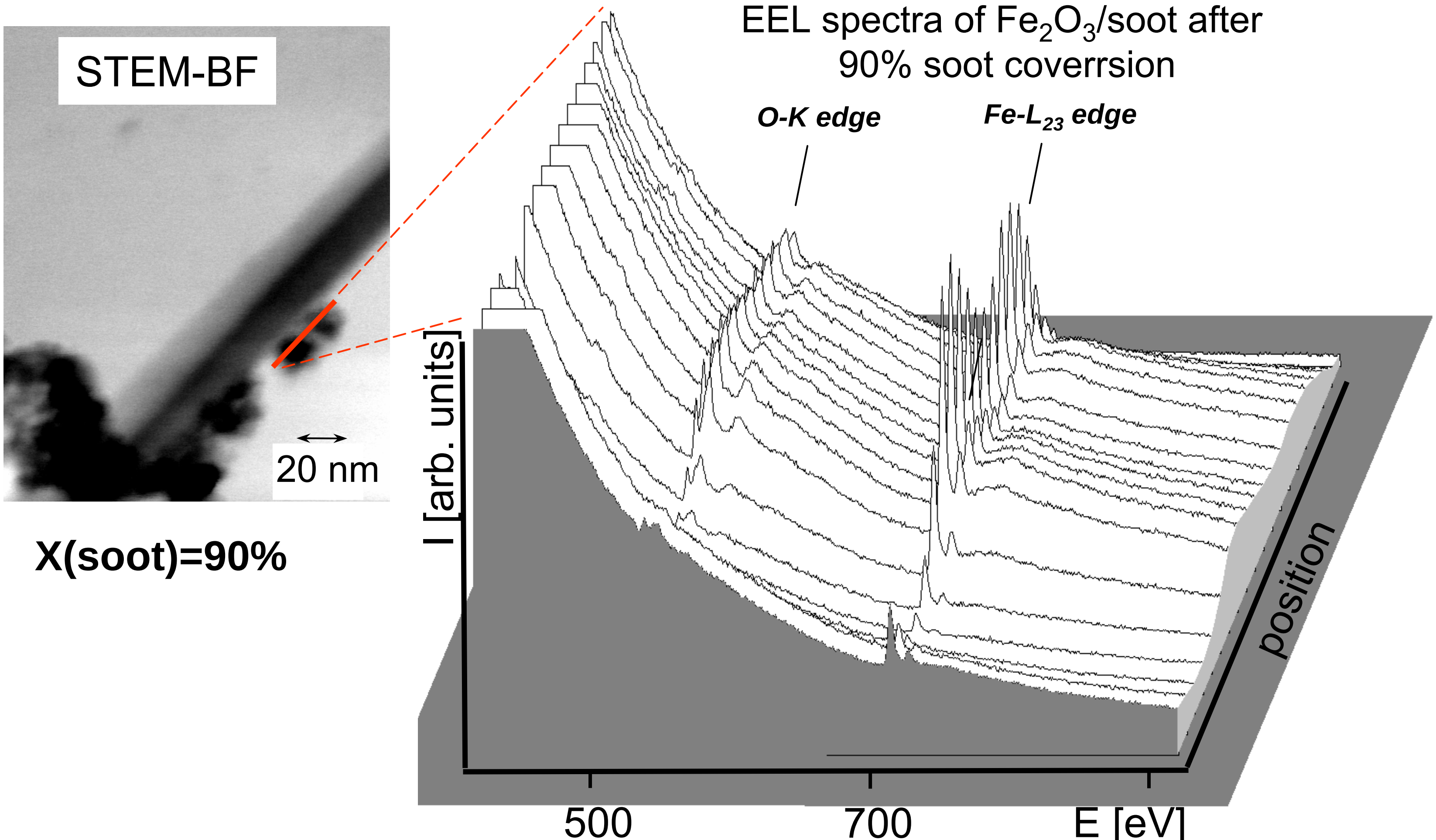
Summary

- Fe_2O_3 catalyst enhances the soot oxidation
- Fe_2O_3 catalyst transfers the gas-phase oxygen to the soot at the contact points
- Gas-phase oxygen adsorbs dissociatively on O vacancies and migrates on the Fe_2O_3 surface to the contact points
- Contact between catalyst and soot maintains up to high conversion levels
- Catalyst is not directly involved in the soot/oxygen reaction

Outlook and current activities

- **Study of the interaction between soot and Fe_2O_3 in the sub-nm range**



X(soot)=90%

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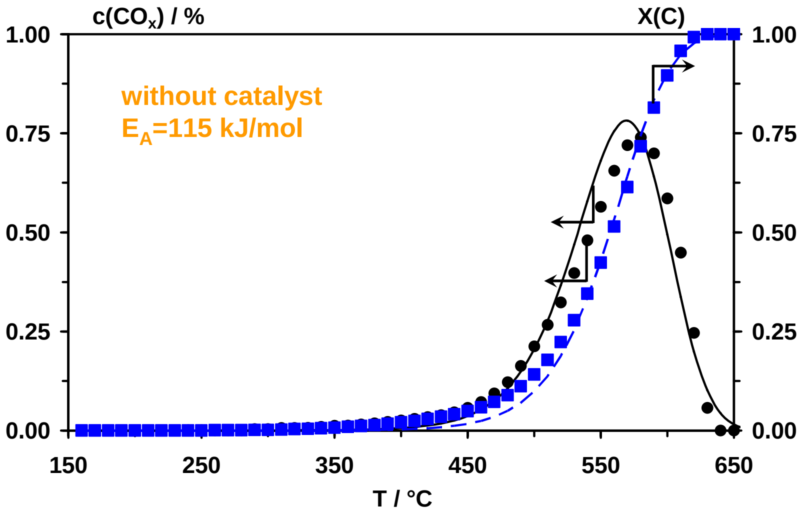
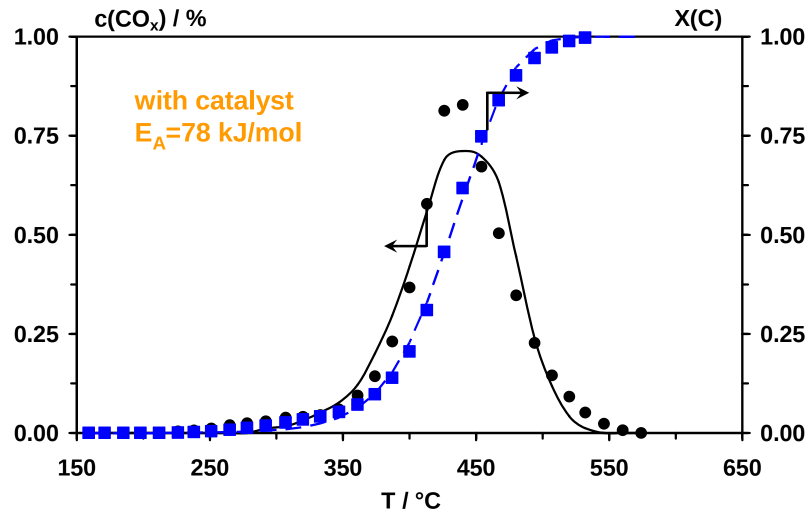
- **Kinetic modelling**

$$\beta \cdot \frac{dX}{dT} = A \cdot e^{\left(-\frac{E_A}{RT}\right)} \cdot \lambda \cdot S_0 \cdot m_0 \cdot (1-X) \cdot \sqrt[3]{1+f \cdot X} \cdot c(O_2)^{n_{O_2}}$$





- **Development of improved Fe_2O_3 catalysts**

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