**EXACT**  
Project ID: EVK2-CT-1999-00053  
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### Effects of the oxidation of aromatic compounds in the troposphere

**From** 2000-02-01 to 2003-01-31

#### Project details

<table>
<thead>
<tr>
<th><strong>Total cost:</strong></th>
<th>EUR 1 096 100</th>
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<tbody>
<tr>
<td><strong>EU contribution:</strong></td>
<td>EUR 899 500</td>
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<td><strong>Coordinated in:</strong></td>
<td>United Kingdom</td>
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<td><strong>Topic(s):</strong></td>
<td>1.1.4.-2. - Key action Global Change, Climate and Biodiversity</td>
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<tr>
<td><strong>Funding scheme:</strong></td>
<td>CSC - Cost-sharing contracts</td>
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#### Objective

Problems to be solved  
Aromatic compounds are emitted to the atmosphere from transport and industrial sources and oxidised in the troposphere. This process has a substantial impact on the formation of ozone and of photochemical smog on a European scale, and on the oxidising capacity of the atmosphere and hence on global warming. The oxidation of aromatic compounds also leads to the formation of secondary aerosols, with impacts on health and on climate. A quantitative understanding of the chemical mechanisms for oxidation of the major aromatic compounds is needed for the construction of models for both predictive and legislative applications and for the assessment of environmental impact. Recent laboratory studies have demonstrated considerable uncertainties in our present understanding of the atmospheric oxidation of aromatics and have seriously questioned our ability to assess the atmospheric impact of aromatic compounds. The major aim of the project is a detailed laboratory investigation of the mechanism and the construction and application of a model, based on the experimental results, to assess the atmospheric impact of aromatic emissions on European and global scales.

Scientific objectives and approach.
The project consists of four main components: In the laboratory experiments, laser flash photolysis is used to probe the chemistry of the early stages of the oxidation process, using absorption spectroscopy. A key element is the behaviour of adducts formed by the addition of the hydroxyl radical to the aromatic compounds. The subsequent chemistry is probed using photochemical reactor studies, coupled with a range of analytical techniques, such as Fourier transform infrared spectroscopy and gas chromatography. A key component of the strategy is the synthesis of important intermediates to test the hypotheses that are developed. The overall description of the oxidation of the major volatile organic compounds emitted to the atmosphere is contained in a master chemical mechanisms (MCM). The experimental results allow revision of the aromatic component of the MCM, which is then used to design experiments to test the proposed mechanisms. These experiments are conducted in the European Photochemical Reactor (EUPHORE) at Valencia in Spain. The EUPHORE experiments are conducted under conditions close to those pertaining in the atmosphere and provide a credible test of the MCM and hence of the laboratory experiments. Crucial experiments include the yield of ozone in aromatic oxidation, but the extensive instrumentation in EUPHORE permits a wide range of detailed experimental checks on the MCM. In addition, other experiments allow investigation of the formation of secondary organic aerosol. The result of these studies is a validated mechanism for aromatic oxidation, contained within the MCM. This revised MCM is then used in a photochemical trajectory model to assess the impact of aromatic emissions on regional ozone formation in Europe. In addition, it is feasible to use the MCM to assess the effect of aromatic emissions on the formation of secondary organic aerosol and on the chemistry of the free troposphere and hence on global warming.

Expected impacts
It is expected that the results will provide a clear assessment of atmospheric impacts of aromatic compounds. Current studies put the contribution of these compounds to European ozone concentrations at the 30% level, although recent measurements suggest that the atmospheric burden of aromatics is at a higher level than is currently accepted. Thus an accurate assessment of the influence of aromatic compounds is of paramount importance. The photochemical trajectory calculations permit the...
determination of photochemical ozone creation potentials (POCPs) for the aromatics, which provide a quantitative measure of their impact on regional ozone. The POCPs can be used for legislative and predictive purposes. It is more difficult to gain a quantitative assessment of the impact of aromatics on secondary organic aerosol and a key aspect of the project is the development of appropriate tested chemical mechanisms and their application to assess impacts. It is thought that about 30% of urban particles derive from secondary organic aerosol. The importance of particles from a human health perspective demonstrates the relevance of this component of the project. Finally, a more qualitative assessment will be made of the global impact of aromatic oxidation, through the formation of longer lived intermediates that can affect the chemistry in the free troposphere and through the influence of secondary organic aerosol on the formation of cloud condensation nuclei and hence on climate.

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