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# Atmospheric Chemistry - CHE00031H

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- **Department:** Chemistry
- **Module co-ordinator:** Prof. Mat Evans
- **Credit value:** 20 credits
- **Credit level:** H
- **Academic year of delivery:** 2020-21
  - See module specification for other years: [2019-20](#)

## Module will run

**Occurrence**

A

**Teaching cycle**

Autumn Term 2020-21

## Module aims

Human activities lead to the polluting of the atmosphere influencing the quality of the air we breathe, changing the climate and disturbing ecosystems. For example, particulate matter accounts for an average loss of life expectancy of around eight months for every resident of the UK and its economic cost of premature mortality and health service costs amounts to some £16.4 billion per annum. This course is designed to look at the chemical and physical processes important in controlling the concentration of pollutants in the atmosphere both in the gas and aerosol phase and their impact. The course starts with the physics of the atmosphere that determines the movement of air around the planet giving the weather patterns we see every day. It then moves to understand the processes which determine the atmosphere's temperature and so the climate and how this may have changed in the past and may change into the future. The chemistry important in the urban, background and upper atmosphere is discussed both for gas and aerosol phases. Computer models play a central role in our understanding of atmospheric pollution and a range of these models are discussed. The different analytical techniques used to measure the composition of the air on the ground, from aircraft and from space are then presented. Finally, three case studies of how this science has been used to determine policy will be presented covering urban air pollution, stratospheric ozone loss and climate change.

At the end of the course students will understand the complexity of the chemistry and physics that determine the composition of the atmosphere, appreciate the tools available to the atmospheric chemist for understanding the composition of the atmosphere and have a sense of how this science has been used to craft government policy to reduce the impact of human activity on the atmosphere.

## Module learning outcomes

### Met and Physical Climate

- Understanding of the different regions of the atmosphere and the flow of air within the atmosphere.
- Understand the balance of energy and heat in the atmosphere and how this related to climate
- Be able to explain the concepts of radiative forcing, climate sensitivity and climate feedbacks, be able to give examples of different feedbacks and be able to quantitatively understand the impacts
- Understand how a climate model works and the processes it might consider
- Be able to describe a range of predictions that are made for future climates over the next 100 years.

### Tropospheric Chemistry

- Understand the chemistry of ozone in the troposphere through the chemical cycling of Ox, HOx, ROx and NOx.

- Understand why ozone production is non-linear with respect to NO<sub>x</sub> and VOCs.
- Understand some of the complexities of atmospheric organic chemistry
- Understand how an atmospheric chemical mechanism is constructed

#### Stratospheric Chemistry

- Be able to describe the chemistry of ozone in the stratosphere through the use of various Ox cycles and catalytic loss processes involving HO<sub>x</sub>, NO<sub>x</sub>, ClO<sub>x</sub> and BrO<sub>x</sub>.
- Understand the causes of the stratospheric ozone hole.

#### Aerosol chemistry

- Understand the differing health impacts of aerosols
- Understand how aerosols are formed and removed from the atmosphere
- Be able to describe how aerosol sizes vary with composition and source.
- Understand how aerosols influence climate.

#### Measurement and Policy

- Be able to describe how the measurement of air pollution gases and aerosols are made for policy objectives
- Be able to describe how measurements of air pollution gases and aerosols are made for research objectives
- Understand how air quality policy is made in the UK
- Understand how research influences air quality policy.

#### Other learning outcomes

- Be able to use a simple computer model to investigate a set of air quality policy questions
- Be able to write a report suitable for a policymaker.

## Module content

### **Meteorology and Physical Climate**

- *Lecture 1: Radiative balance of the atmosphere. (1-hour MJE)*
  1. Incoming UV outgoing IR balance
  2. Albedo
  3. Greenhouse effect
  4. Optical thickness
  5. Nonlinear response of radiation to CO<sub>2</sub>
  6. IPCC radiation balance.
- *Lecture 2: Atmospheric structure (1-hour ACL)*
  1. Convection, atmospheric pressure gradient, hydrostatic approximation
  2. Atmospheric pressure gradient
  3. Lapse rate
- *Lecture 3: Atmospheric structure (1-hour ACL)*
  1. Temperature profile
  2. Dry adiabatic lapse rate

## 3. Stability.

• *Lecture 4: Atmospheric Circulation (1-hour ACL)*

1. Buoyancy, Brunt Vaisala
2. Circulation, Coriolis, Pressure gradient force, Drag.

• *Lecture 5: Radiative Forcing (1-hour MJE)*

1. Definition of radiative forcing
2. Radiative forcing of different components
3. History of IPCC radiative forcing graphs
4. Climate Sensitivity
5. Feedbacks
6. Calculating Climate Sensitivity
7. Estimating Climate Sensitivity

• *Lecture 6: Climate Models (1-hour MJE)*

1. Modules and submodules
2. Evolution of climate models with time
3. Differential equations. Conservation laws.
4. Weather, chaos and climate
5. Multimodel means

• *Lecture 7: Future Predictions. (1-hour MJE)*

1. Scenario generation. SRES, RCPs
2. Future predicted concentrations
3. Predicted radiative forcings
4. Predicted temperatures / sea level rise / ice extents
5. Geo-engineering

## • Workshop 1: Unassessed. Aspects of Meteorology and Physical Climate (2-hours MJE)

**Chemistry of Gases in the troposphere and stratosphere**• *Lecture 8: Stratospheric chemistry (1-hour LJC)*

1. Chapman chemistry
2. NO<sub>x</sub>, HO<sub>x</sub> chemistry
3. Ozone hole discovery

• *Lecture 9: Stratospheric chemistry (1-hour LJC)*

1. ClO<sub>x</sub>, BrO<sub>x</sub> Chemistry
2. Heterogeneous chemistry
3. CFCs

• *Lecture 10: Stratospheric policy (1-hour LJC)*

1. Montreal protocol
2. Successes
3. Future directions

- *Lecture 11: Tropospheric Chemistry O<sub>3</sub>/NO<sub>x</sub> (1-hour MJE)*
  1. Ozone budget
    1. Ozone deposition
    2. Strat Trop Exchange
    3. Ozone production
    4. Ozone loss
  2. Chemistry of ozone loss
  3. Chemistry of ozone production
  4. Nitrogen oxides
    1. Sources
    2. Sinks
    3. Budget
  
- *Lecture 12: Tropospheric Chemistry Radicals/VOCs (1-hour MJE)*
  1. Radicals
    1. Sources
    2. Sinks
    3. OH radical
    4. High NO<sub>x</sub>
    5. Low NO<sub>x</sub>
  2. VOCs
    1. Typical VOCs in the atmosphere
    2. VOC sources
    3. VOC sinks
    4. Methane
  
- *Lecture 13: Tropospheric Chemistry O<sub>3</sub> production (1-hour MJE)*
  1. O<sub>3</sub> production and loss
    1. O<sub>3</sub> as a function of NO<sub>x</sub>. Non-linear production
    2. Ozone isopleths
  2. LA vs London
  3. Differing impact of different VOC. POCP
  4. Local vs regional vs global air pollution
  5. Air quality standards
  
- *Lecture 14: Advanced Atmospheric Organic Chemistry (1-hour ARR)*
  1. Relative importance of oxidants
    1. Diurnal profiles and concentrations
    2. VOC speciation and reactivity
  2. OH + alkane chemistry

3. OH + aromatic chemistry
  4. OH + alkene chemistry
  5. NO<sub>3</sub> + alkene chemistry
  6. Ozonolysis
    1. Criegee chemistry
      1. Radical formation
      2. SCI oxidant chemistry
- *Lecture 15: Advanced Atmospheric Organic Chemistry (1-hour ARR)*
    1. Detailed mechanism development - MCM
      1. Construction methodology/framework
      2. Structure Activity Relationships
      3. MCMv3.3.1
    2. Scientific applications
  - *Lecture 16: Advanced Atmospheric Organic Chemistry (1-hour ARR)*
    1. MCM policy applications
      1. Mechanism reduction/parameterisation
    2. POCP
      1. Basis
      2. Trajectory model
      3. Application examples
    3. Chamber evaluation
      1. Use of outdoor chambers (EUROCHAMP)
      2. Chamber specific modelling
        1. Examples - Aromatic chemistry
  - Workshop 2 (Assessed through the take-home exercise) Atmospheric Chemistry Modelling (2-hour MJE)
  - Workshop 3 (Assessed through the take-home exercise) Atmospheric Chemistry Modelling (2-hour MJE)

### **Chemistry of aerosols**

- *Lecture 17: Human health effects from exposure to pollutants. (1-hour JFH)*
  1. Health effect pyramid and chronic/acute effects
  2. Exposure routes and respiratory system
  3. Particles
  4. Ozone
- *Lecture 18: Introduction to aerosols (1-hour JFH)*
  1. Atmospheric impacts of particles
  2. Sources of aerosols
  3. Size classifications
  4. Atmospheric processing and sinks

- *Lecture 19: Physical properties and sinks of aerosols (1-hour JFH)*
  1. Dry and wet deposition
  2. Particle-particle interactions
  3. Volatility and viscosity
- *Lecture 20: Chemical classification of aerosols (1-hour JFH)*
  1. Primary particles - sea salt, minerals, soot
  2. Secondary particles - sulfate, nitrate, intro to SOA
  3. Water particles - PSC (v limited here), contrails
- *Lecture 21: Organic Aerosols (1-hour JFH)*
  1. Sources of organic species
  2. Secondary organic aerosol formation
  3. Biogenic versus anthropogenic
  4. Aerosol Yields and partitioning theory.
- *Lecture 22: Aerosols and climate (1-hour JFH)*
  1. Direct and semi-direct aerosol effects
  2. Indirect aerosol effects
  3. Ice nucleation
  4. Other impacts on weather and climate
- *Workshop 4: Unassessed. Aspects of Aerosol chemistry. (2-hours JFH)*

### **Measurement techniques and policy**

- *Lecture 23: Measurements of gases: Optical techniques (1-hour PME)*
  1. Requirements: accuracy, precision, sensitivity, selectivity
  2. DOAS (LP and MAX)
  3. Cavity techniques (cavity ring down, direct absorption, cavity enhanced)
  4. Chemiluminescence
  5. Laser-induced fluorescence
- *Lecture 24: Measurements of gases: Optical applications and sensors (1-hour PME)*
  1. Satellite instruments
  2. Measurements of chemical families using conversion inlets (e.g. NO<sub>y</sub>)
  3. OH reactivity
  4. Low-cost sensors (optical, electrochem and metal oxide)
- *Lecture 25: Measurements of gases: Separation and Mass spectrometric techniques (1-hour JL)*
  1. GC FID and MS
  2. 2d GC
  3. PTR/CIMS (ToF?)
  4. Offline methods e.g. cans, diffusion tubes
- *Lecture 26: Measurements of gases: Fluxes (1-Hour JL)*
  1. Eddy covariance technique

2. Mass balance
- *Lecture 27: Measurements of particles: Network instrumentation (1-Hour JFH)*
    1. Introduction to the network in UK and regulated species
    2. Aerosol inlets
    3. TEOM and FDMS
    4. BAM
    5. Gravimetric
  - *Lecture 28: Measurements of particles: Research instruments for composition (1-hour JFH)*
    1. Filter samples and chromatography/mass spectrometry
    2. AMS
      1. Aerodynamic lens
      2. Instrument components
      3. Data analysis
      4. Atmospheric data
      5. Factor analysis
  - *Lecture 29: UK Air Quality Policy (1-hour SM)*
    1. Historic legislation, the Clean Air Act
    2. European Air Quality Directives
    3. The wider policy picture
  - *Lecture 30: UK Monitoring for Policy (1-hour SM)*
    1. UK ambient AQ networks - inc. challenges, equivalence, site classification & location
    2. Trends & links to policy [need to check overlaps with others, could be across EU]
    3. Ecosystems impacts
    4. Monitoring for ecosystems impacts
    5. Future of monitoring - challenges and opportunities
  - *Lecture 31: Role of Research in Policy Development (1-hour SM)*
    1. The compliance challenge - Case study: NO<sub>2</sub> issue
    2. The evidence behind this issue
      1. Trends in concentration and emissions
      2. Emissions measurements & NAEI
      3. Remote Sensing
      4. PEMS
    3. Failure of Euro standards
    4. The National Plan for NO<sub>2</sub>
    5. Future challenges
  - Workshop 5: Unassessed. Aspects of Measurements and Policy chemistry. (2-hours SM)

## Assessment

Task	Length	% of module mark
<b>24 hour open exam</b> Atmospheric Chemistry	N/A	80
<b>Practical</b> Computer Practical	N/A	20

## Special assessment rules

None

## Additional assessment information

The exam has 2 compulsory 25 mark questions. This will assess all of the course other than the "Chemistry of Gases in the troposphere and stratosphere" section. The two exam questions will assess all of the other sections of the course. Each exam question can select material to examine from any of the other sections.

The computer practical assessment asks the student to imagine that they are an environmental consultant writing a report on the air quality in a city. Each student is allocated a different city and given a unique set of conditions for that city. They are then expected to answer a set of questions about the air quality in that city using an atmospheric computer model in the form of a report to the mayor of the city. This is completed as a take-home exercise with an electronic submission two weeks after the last workshops. To support this activity there are 2 computer practical computer practicals which run through the use of the model and some tools and techniques for exploiting it. The report is graded on the basis of the quality of the presentation and the scientific answers to the questions.

## Reassessment

Task	Length	% of module mark
<b>24 hour open exam</b> Atmospheric Chemistry	N/A	80
<b>Practical</b> Computer Practical	N/A	20

## Module feedback

Closed exam results with per-question breakdown are returned to the students via supervisors within 5 weeks (as per special approval by the University Teaching Committee). Outline answers are made available via the Chemistry web pages when the students receive their marks, so that they can assess their own detailed progress/achievement. The examiners' reports for each question are made available to the students via the Chemistry web pages.

Individual written feedback will be given for the assessed aspect if the computer practical work within 5 weeks of submission.

Answers and comments to the 3 computer workshops are provided the day after the workshop has occurred.

## Indicative reading

Introduction to Atmospheric Chemistry, by [Daniel J. Jacob](#), Princeton University Press, 1999

Atmospheric Chemistry and Physics: From Air Pollution to Climate Change by John H. Seinfeld and Spyros N. Pandis, Wiley, 2016

Atmospheric Chemistry, Ann Holloway and Richard Wayne, Royal Society of Chemistry, 2010



Analytical Techniques for Atmospheric Measurement, Dwayne Heard, Blackwell publishing, 2008

The information on this page is indicative of the module that is currently on offer. The University is constantly exploring ways to enhance and improve its degree programmes and therefore reserves the right to make variations to the content and method of delivery of modules, and to discontinue modules, if such action is reasonably considered to be necessary by the University. Where appropriate, the University will notify and consult with affected students in advance about any changes that are required in line with the University's policy on the [Approval of Modifications to Existing Taught Programmes of Study](#).

## Coronavirus (COVID-19): changes to courses

The 2020/21 academic year will start in September. We aim to deliver as much face-to-face teaching as we can, supported by high quality online alternatives where we must.

Find details of the measures we're planning to protect our community.

[Course changes for new students](#)