# Chemistry Working Group

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## CWG's Prospective Roles in Community and SMG

- Act as First Point of Contact for UKCA Community on matters concerning chemistry
  - Representing community in UKCA SMG
  - Coordinating mechanism/model development
  - Working with other UKCA WGs
  - Networking with "neighbouring" communities (such as, dry deposition, land surface, etc.)
- Act as focal points in SMG on matters concerning chemistry
  - Coordinating ongoing science
    - Minimizing potentially overlapping efforts
  - Identifying research priorities in the UKCA chemistry community
    - Exploiting synergies, connecting research groups
  - Seeking out new areas of research in chemistry modelling
    - Identifying hot topics and emerging fields of research
  - Facilitating integration in UKCA

#### What are "Matters Concerning Chemistry"? - a snapshot

- Surface and 3D emissions
  - Probably outside our scope this is a choice for users
  - Simplifying implementation of new emissions in UKCA under discussion elsewhere
- Photolysis
  - FastJx maintenance of code, implementation of updates
- Chemical reactions
  - Underpinning data: reaction rate coefficients, photolysis cross-sections, uptake coefficients
  - Maintenance of numerical solvers
    - ASAD will the Backward Euler continue?
- Deposition schemes
  - Surface dry deposition
  - Wet removal
- Maintenance of code
- Evaluation of chemistry

#### UKCA Implementations - many and diverse - where next?

- UKCA standalone versions
  - UKCA box model
  - UKCA column model
- UKCA VM
  - Facilitating development and testing of new code
- UKCA in the UM
  - Needs to satisfy divergent roles of chemistry in Earth system, climate and air quality modelling
    - Variable degree of complexity in the chemistry
    - Emphasis on different species with potentially divergent mechanisms
      - MO GAX.y configurations
      - UKESM configurations
      - Existing schemes such as ExTC, Backward-Euler solvers
  - Implementing and review (by the community?) of new schemes
    - Whole atmosphere chemistry schemes
    - Air quality schemes

#### What are we looking to improve? (suggestions only, feedback welcome)

- The UKCA VM has been a fantastic addition to development
  - o How do we maintain it?
  - How do we update it for future releases?
- Model integrations are expensive and time-consuming
  - Could we do a better job of archiving output for community use?
- How do we let people know what's going on and help them to get involved?
  - Improving information flow with the Wiki?
  - Regular telecons? Side meetings?
  - Networking beyond Chemistry
    - other UKCA WGs
    - other WGs with Close Relation to Chemistry (e.g., dry deposition, land surface, etc.)

### What are we thinking about?

- Near-term (< 1 year)</li>
  - Gathering intelligence (community consultation); some suggested topics for discussion :
    - Adding CRI as an option for UKCA
    - Implementing Heterogeneous chemistry diagnostics
    - Investigating how to facilitate further updates to FastJx in UKCA
  - Leveraging opportunities for networking (CWG BoG)
    - Improving UKCA evaluation suite (collaboration with <u>E</u>valuation <u>W</u>orking <u>G</u>roup)
- Mid-term (1 to 3 years)
  - Establishing UKCA experiment repository
  - Releasing UKCA standalone (box/column) model
- Long-term (> 3 years)
  - Database of reaction data
  - Automatic mechanism/code generation



# For all of this WE NEED YOUR INPUT!



contact the CWG at

cwg.ukca@gmail.com

Join CWG at Slack

https://cwgukca.slack.com

(email us for an invitation)

or email your suggestions/requests/concerns directly to

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