School of Chemical and Process Engineering
Faculty Of Engineering

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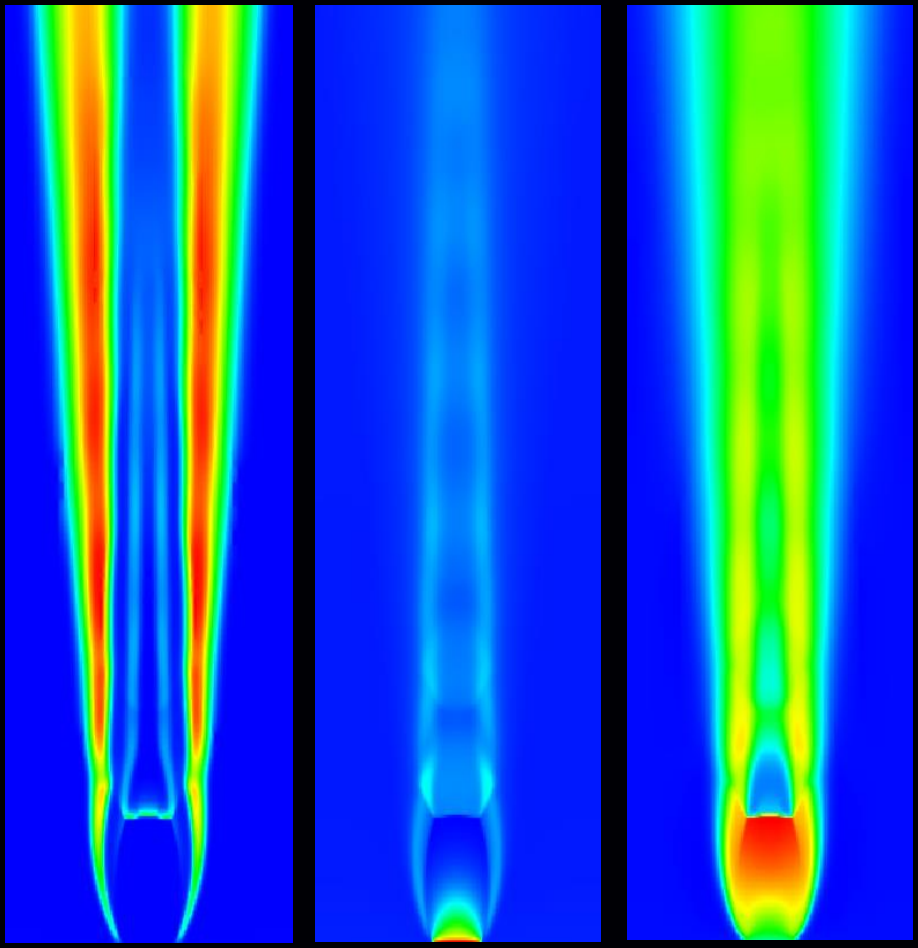
Numerical modelling of turbulence and heat transfer phenomena in accidental CO_2 pipeline releases



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Overview

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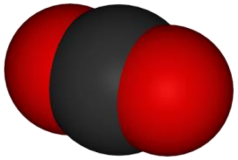
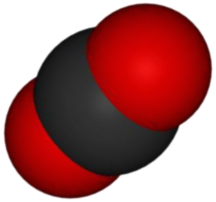
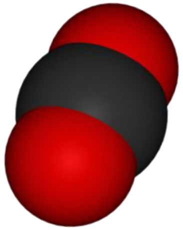
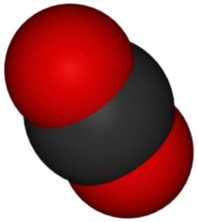
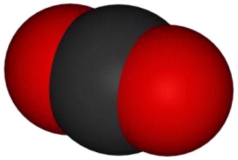
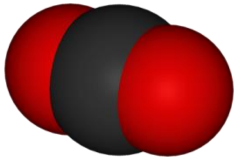
- **Introduction – Work in context**
- **CFD Code**
  - **Adaptive mesh refinement**
  - **Turbulent flow calculations**
  - **Turbulence models and compressibility corrections**
- **Work in Progress**
  - **Multi-component, multi-phase thermodynamics**
  - **Heat transfer modelling**
  - **Particle modelling**

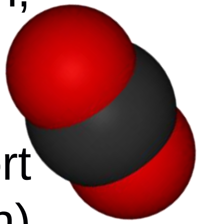






Introduction – Work in context



- Deployment of a complete carbon capture and storage chain requires the implementation of safe, reliable, and cost-efficient technologies to effect the transmission of high-density CO_2.

- Upon release, 10% concentration will cause unconsciousness within 1 minute. 20% concentration is instantaneously fatal. Release and dispersion characteristics must be known for planning, design, and legislation.

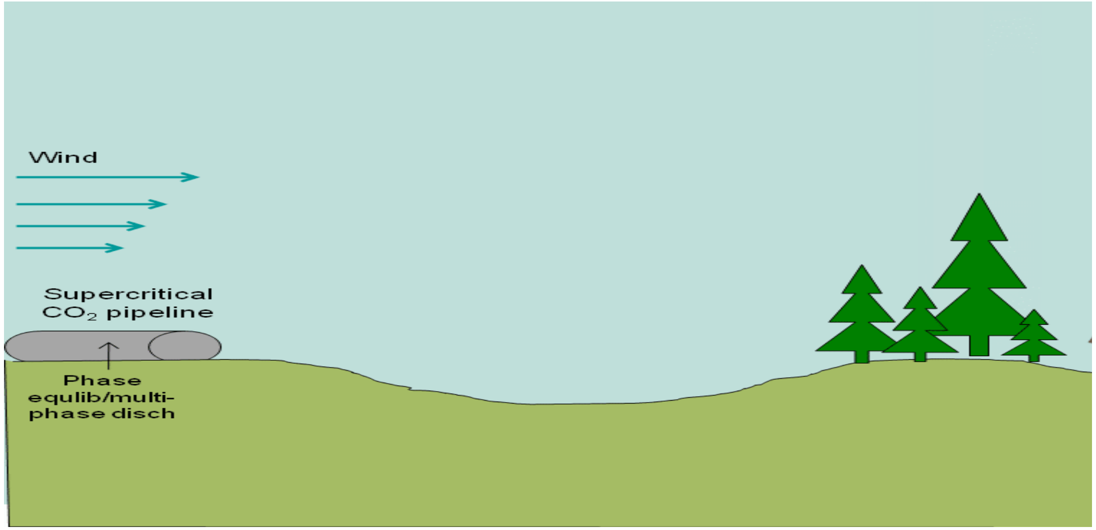


- Complex physics are observed in a release of CO_2 from a transport pipeline. High-pressure CO_2 release (accidental or blow-down) would be a highly under-expanded sonic jet, displaying typical flow phenomena such as stationary Mach discs and shock-diamonds.

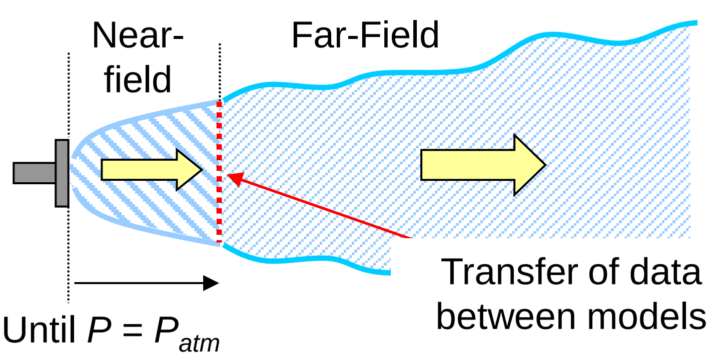
- To describe such a system, an equation of state representing the thermodynamic behaviour of all three phases must be integrated with a model for compressible turbulence.

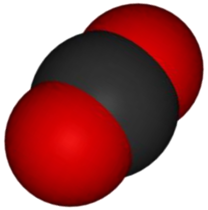
Introduction – Work in context

Schematic representation of CO_2 pipeline release and dispersion scenario:



Integration of numerical models:





CFD Code

Calculations of turbulent flow field.

- Conservative, upwind, finite volume code solving the Reynolds-averaged Navier-Stokes conservation equations for mass, momentum, total energy, mean of mixture fraction. An additional transport equation required for solid phase mass fraction of CO_2.

- Adaptive Mesh Refinement with a hierarchy of grids – Solution computed on all grids. Mesh is refined where solution varies rapidly.

- For shock calculations, we use an HLL (Harten, Lax, van Leer) Riemann solver.

- Coordinates: axisymmetric cylindrical polar.

CFD Code

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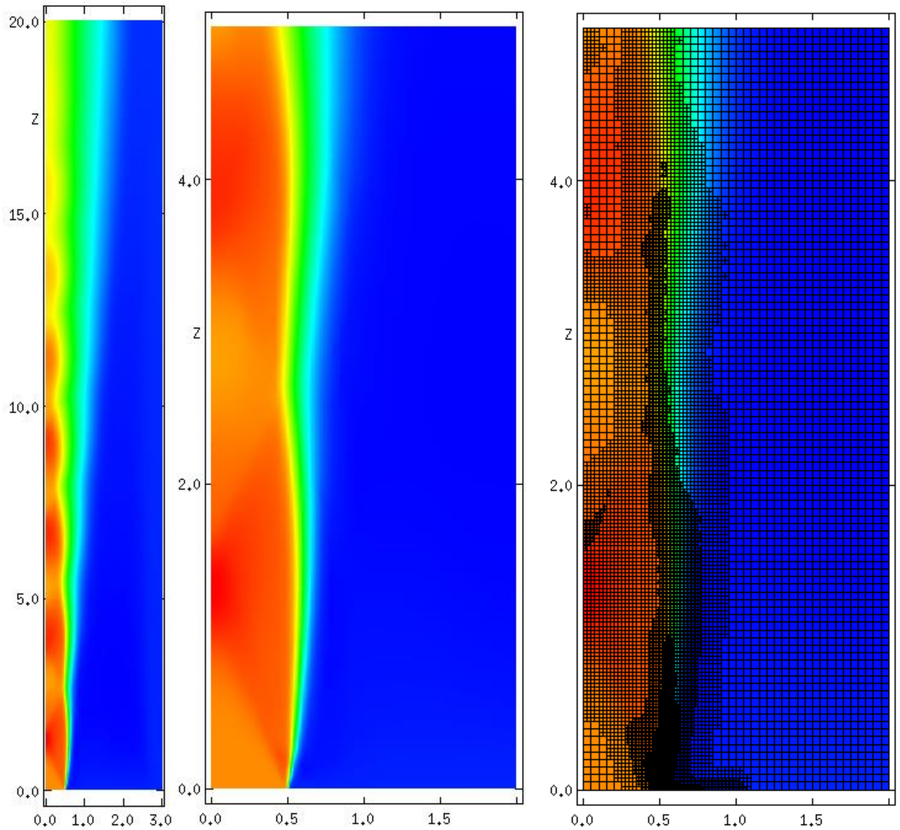
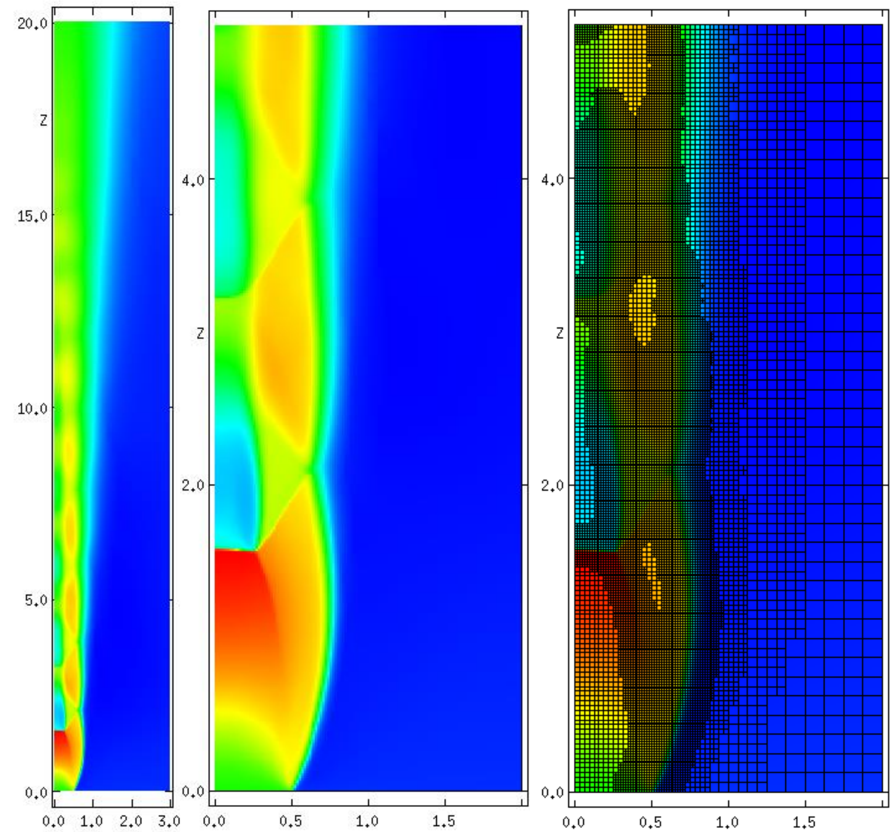
Adaptive Mesh Refinement (AMR)



Moderately Under-expanded



Highly Under-expanded

Adaptive mesh refinement grid mapped onto mean velocity predictions in the near-field region of two under-expanded air jets

CFD Code – Turbulence Modelling

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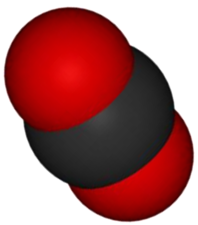
k-ε turbulence model of Jones and Launder (1972).

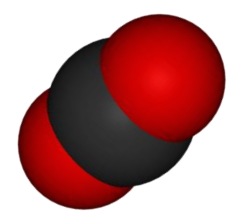
- Boussinesq approximation used to model the Reynolds-stress components.



$$\bar{\rho}u_i''u_j'' = \frac{2}{3}\delta_{ij}\left(\bar{\rho}k + \mu_t \frac{\partial \tilde{u}_k}{\partial x_k}\right) - \mu_t\left(\frac{\partial \tilde{u}_l}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_l}\right)$$

- Here, the turbulence viscosity is represented by a function of the turbulence kinetic energy by:

$$\mu_t = C_\mu \bar{\rho}\frac{k^2}{\varepsilon} \qquad C_\mu = 0.09$$



CFD Code – Turbulence Modelling

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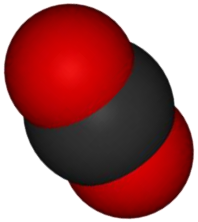
k-ε turbulence model modified using the Sarkar correction for compressibility.

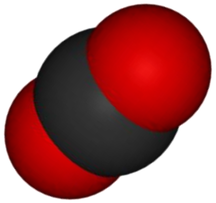
- Compressibility reduces mixing due to enhanced turbulence dissipation.

- Corrections are introduced to the turbulence dissipation rate and turbulence viscosity as a function of Mach number.



- Compressible dissipation rate: $\varepsilon = \alpha M_{\tau}^{2} \varepsilon_{s}$

- Turbulence viscosity: $\mu_t = C_{\mu} \rho \dfrac{k^2}{(1 + M_{\tau}^{2})\varepsilon}$ and $C_{\mu} = 0.09$



CFD Code – Turbulence Modelling

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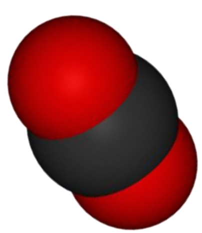
Reynolds-stress transport model

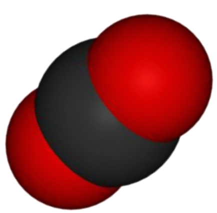
- Reynolds stress transport equation now implemented for turbulence closure.

$$\frac{\partial}{\partial t}\left(\bar{\rho}u_i''u_j''\right)+\frac{\partial}{\partial x_k}\left(\bar{\rho}u_i''u_j''\tilde{u}_k\right)=C_s\frac{\partial}{\partial x_k}\left(\tau\bar{\rho}u_k''u_l''\frac{\partial}{\partial x_l}u_k''u_l''\right)+P_{ij}+A_{ij}-\frac{2}{3}\delta_{ij}\bar{\rho}\varepsilon$$

- Historically, efforts are centered upon modelling the redistribution of stresses in the Pressure-strain correlation

- Correlation can be split into a ‘slow’ and a ‘rapid’ part. Ignoring the ‘rapid’, Rotta (1951) defines it to be:





CFD Code – Turbulence Modelling

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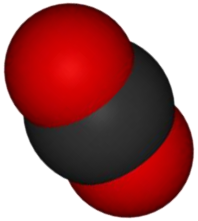
Reynolds-stress transport model

- Rotta (1955)

$$A_{ij} = -C_1 \varepsilon b_{ij} + \cancel{A_{ij}^{rapid}}$$

- Khlifi and Lili (2011)



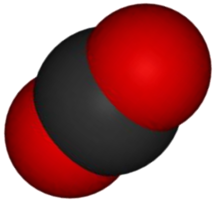
$$A_{ij} = -C_1 \left(1 - \beta M_\tau^2\right) \varepsilon b_{ij} + \cancel{A_{ij}^{rapid}}$$

- Jones and Musonge (1988)

$$A_{ij} = -C_1 \varepsilon \left(\frac{\bar{\rho} u_i'' u_j''}{k} - \frac{2}{3} \delta_{ij} \bar{\rho} \right) + C_2 \delta_{ij} \bar{\rho} u_i'' u_j'' \frac{\partial \tilde{u}_k}{\partial x_l} - C_3 P_{ij} + C_4 \bar{\rho} k \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) + C_5 \bar{\rho} u_i'' u_j'' \frac{\partial \tilde{u}_l}{\partial x_l}$$

$$+ C_6 \left(\bar{\rho} u_k'' u_j'' \frac{\partial}{\partial x_k} (\tilde{u}_k) + \bar{\rho} u_k'' u_i'' \frac{\partial}{\partial x_j} (\tilde{u}_k) \right) + C_7 \bar{\rho} k \delta_{ij} \frac{\partial \tilde{u}_l}{\partial x_l}$$

- Gomez and Girimaji (2013)



$$A_{ij} = -C_1 \left(M_t\right) b_{ij} + \sum_k C_k \left(M_g\right) T_{ij}^k$$

CFD Code – Turbulence Modelling Validation

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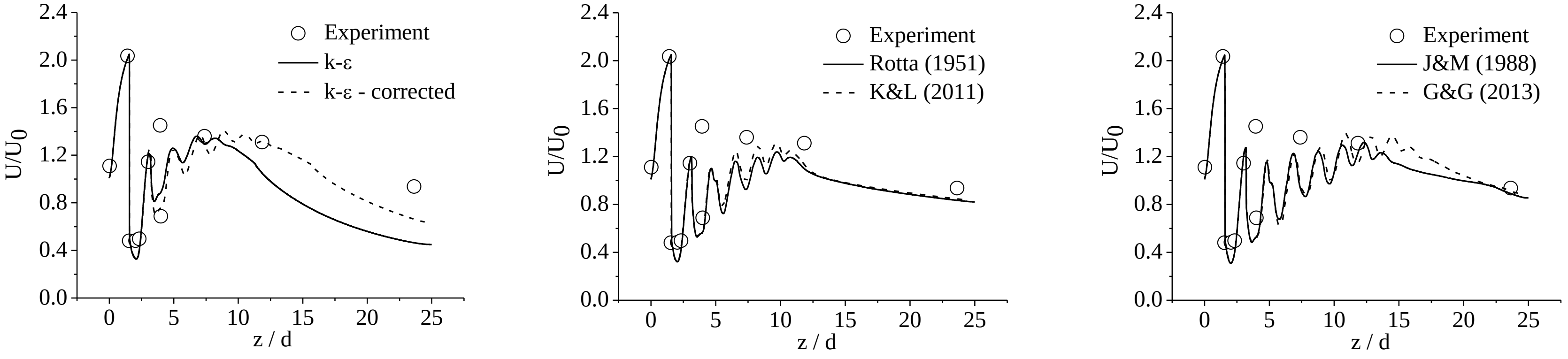
Example of validation case: Donaldson and Snedecker (1971) highly under-expanded air jet normalised velocity predictions with and without corrections



Corrected models validated for cases of moderately and highly under-expanded jets

Conclusions

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- The performance of the axi-symmetric model with various turbulence closures has been assessed and validated using experimental data for under-expanded air jets. Initial calculations show excellent agreement with experiment.

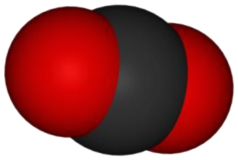
- Reynolds-stress model qualitatively and quantitatively reproduces experimental data well, and outperforms the two-equation model although a slight over-prediction of jet spreading rate remains.

Work in Progress

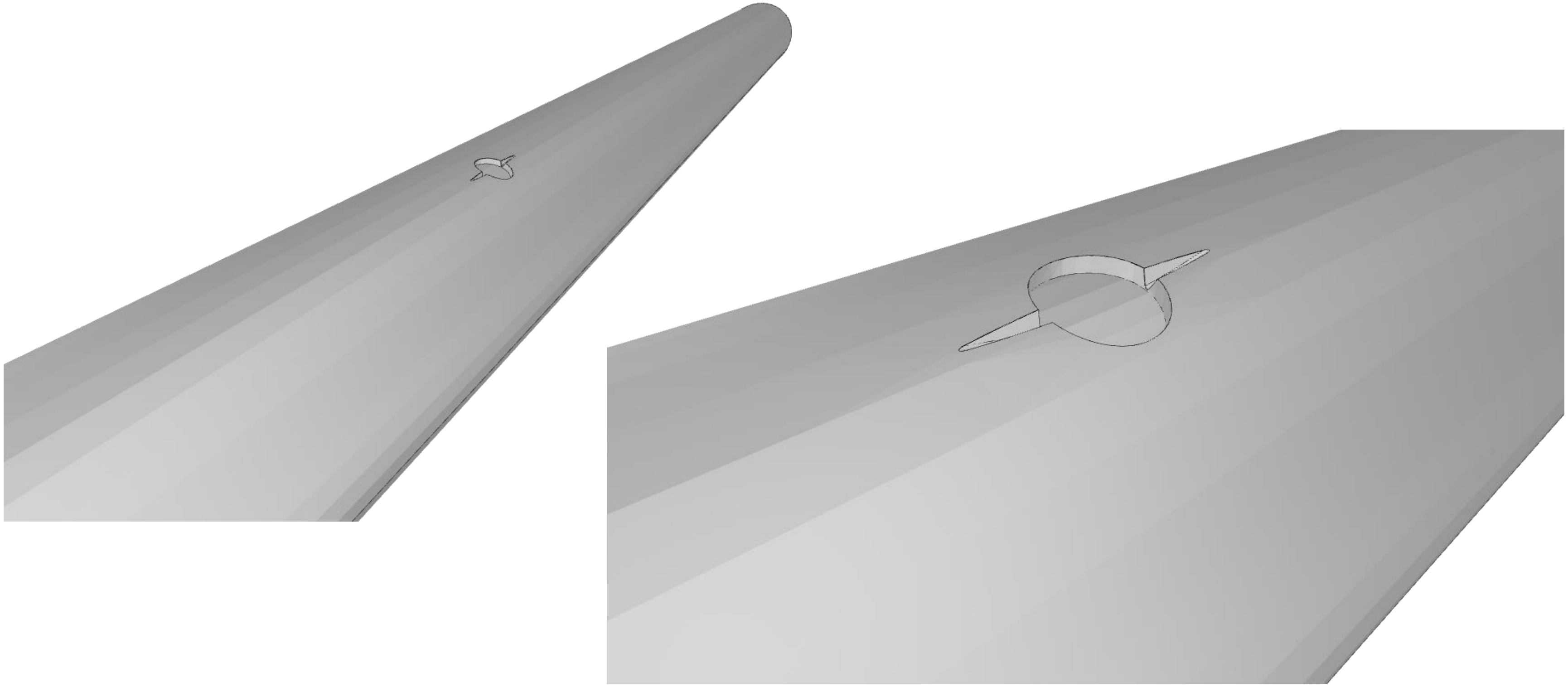
- Integration of compressible turbulence closures now being undertaken with models for:

  - Thermodynamics for multi-component impure CO_2.
  - Conjugate heat transfer to model phenomena at a pipe/fluid interface in the vicinity of a crack.
  - Solid/liquid particle behaviour with respect to condensation, evaporation, and agglomeration.

- The code has been developed for application to full three-dimensional calculations of realistic crater-type scenarios.



Heat transfer modelling – Pre-formed crack



- Pre-formed puncture and crack machined by partners OCAS, Belgium
  - 5 mm diameter

Heat transfer modelling – Experiments

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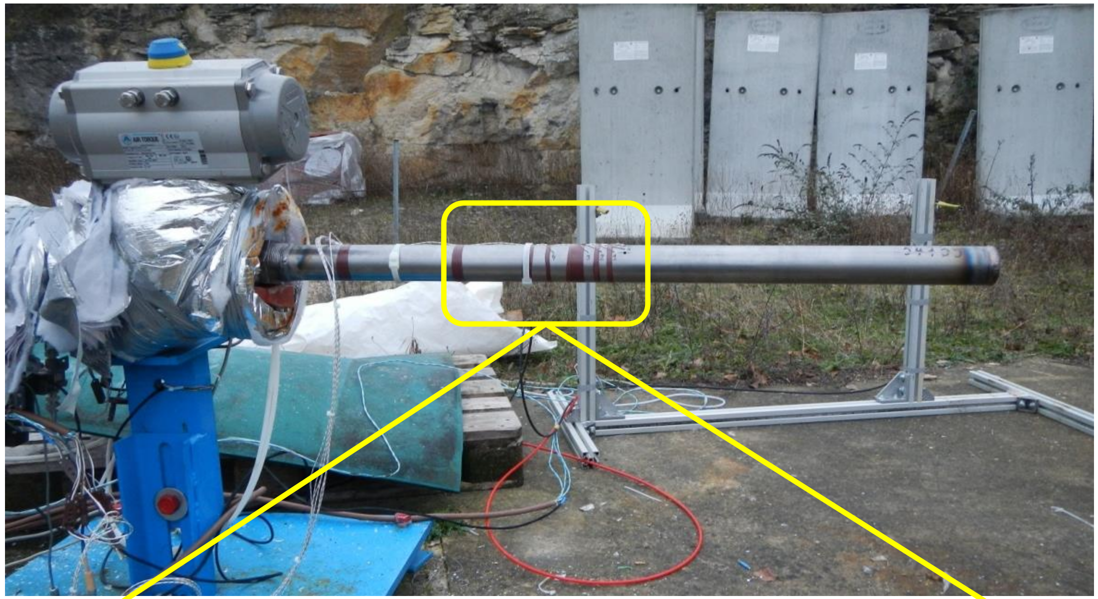
6 mm and 12 mm Punctures also investigated



Heat transfer modelling – Mesh geometry

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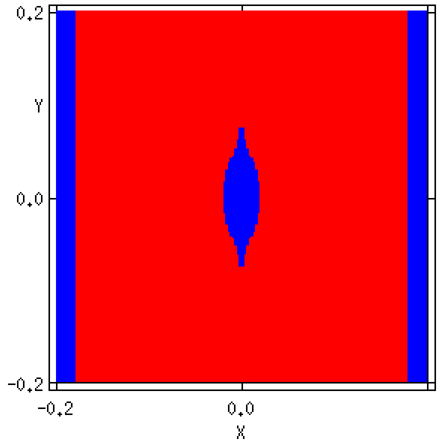

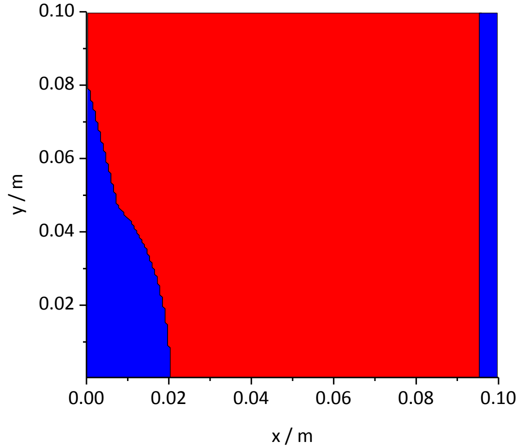

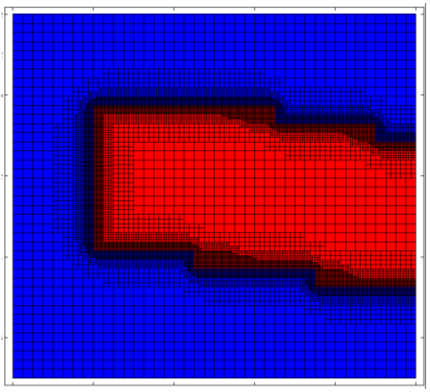

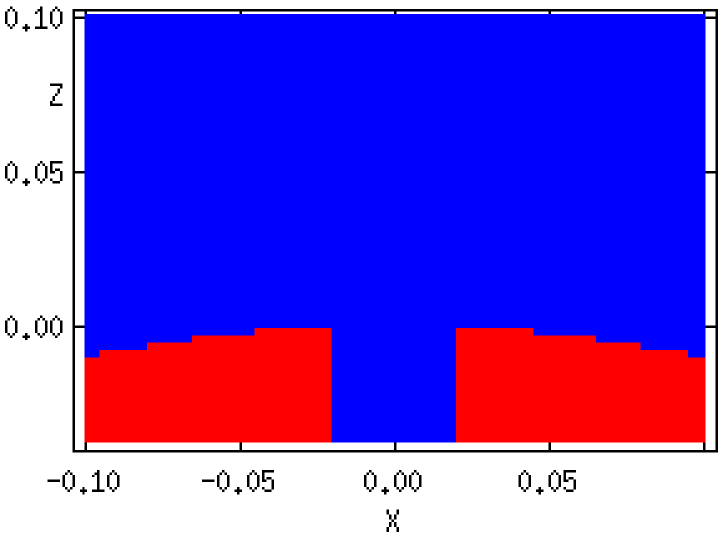

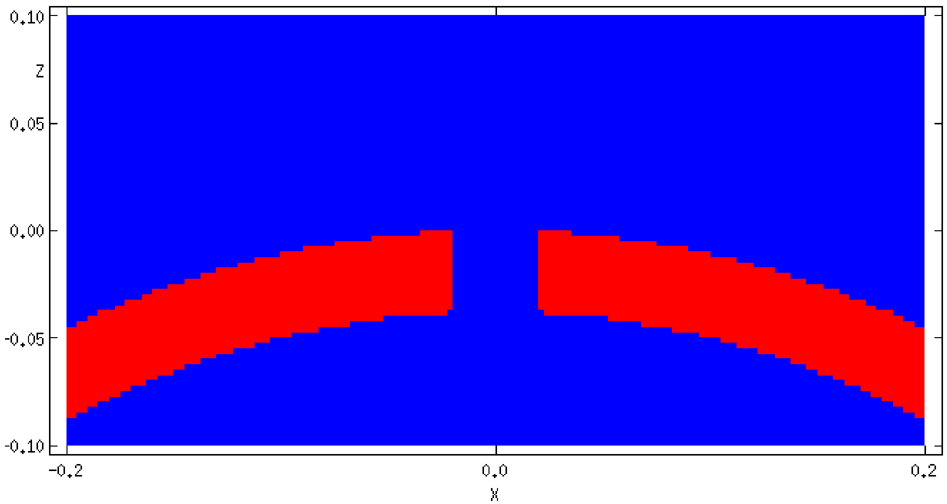

Heat transfer modelling – Preliminary results

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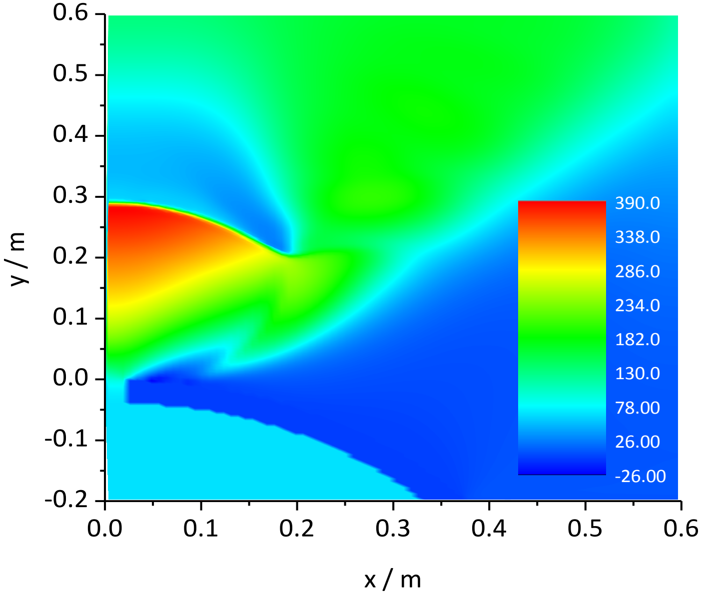
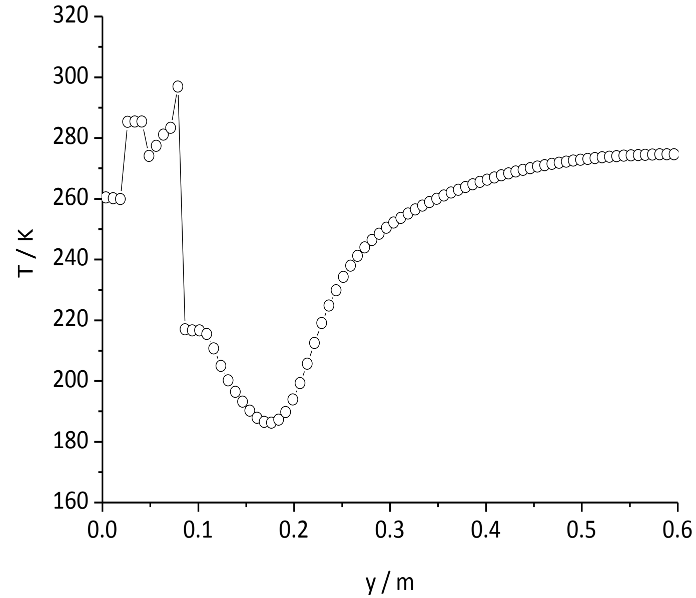
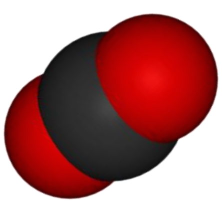
Sample calculation – Initial conditions provided at specific temporal location by UCL



Total velocity prediction



Axial temperature profile of pipe originating at crack centre



Acknowledgements & Disclaimer

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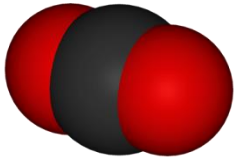

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