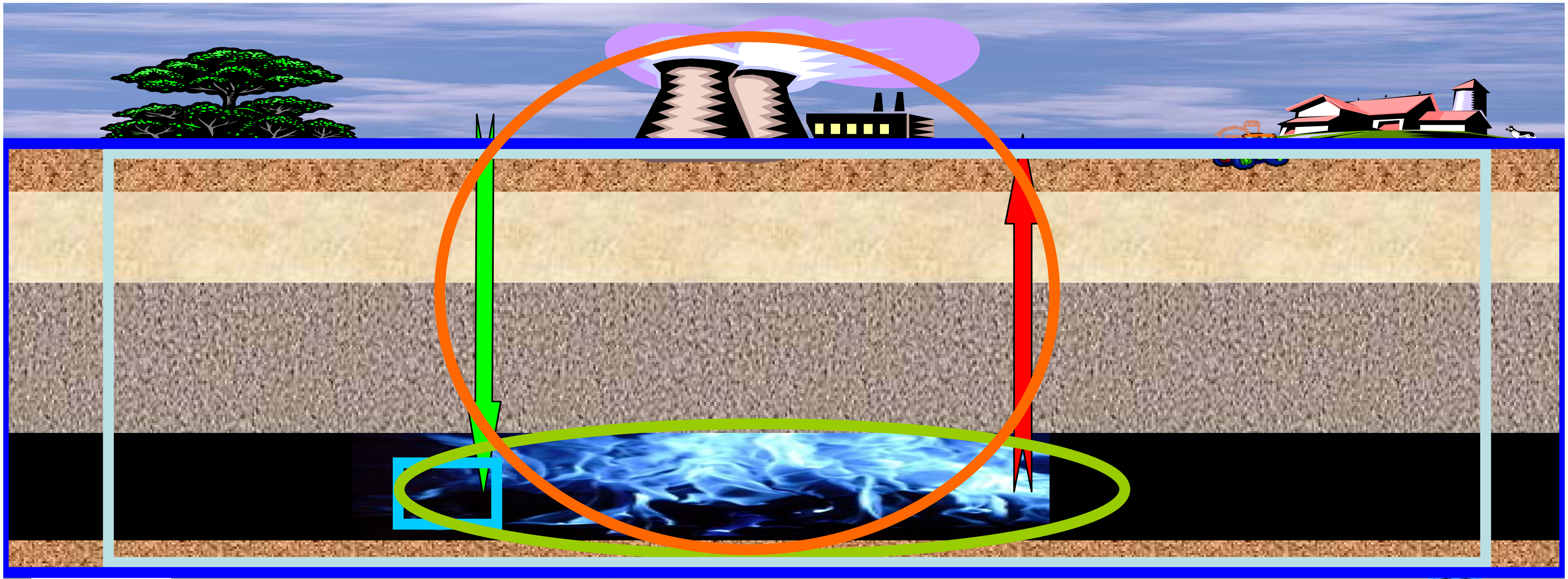

UCG Modelling

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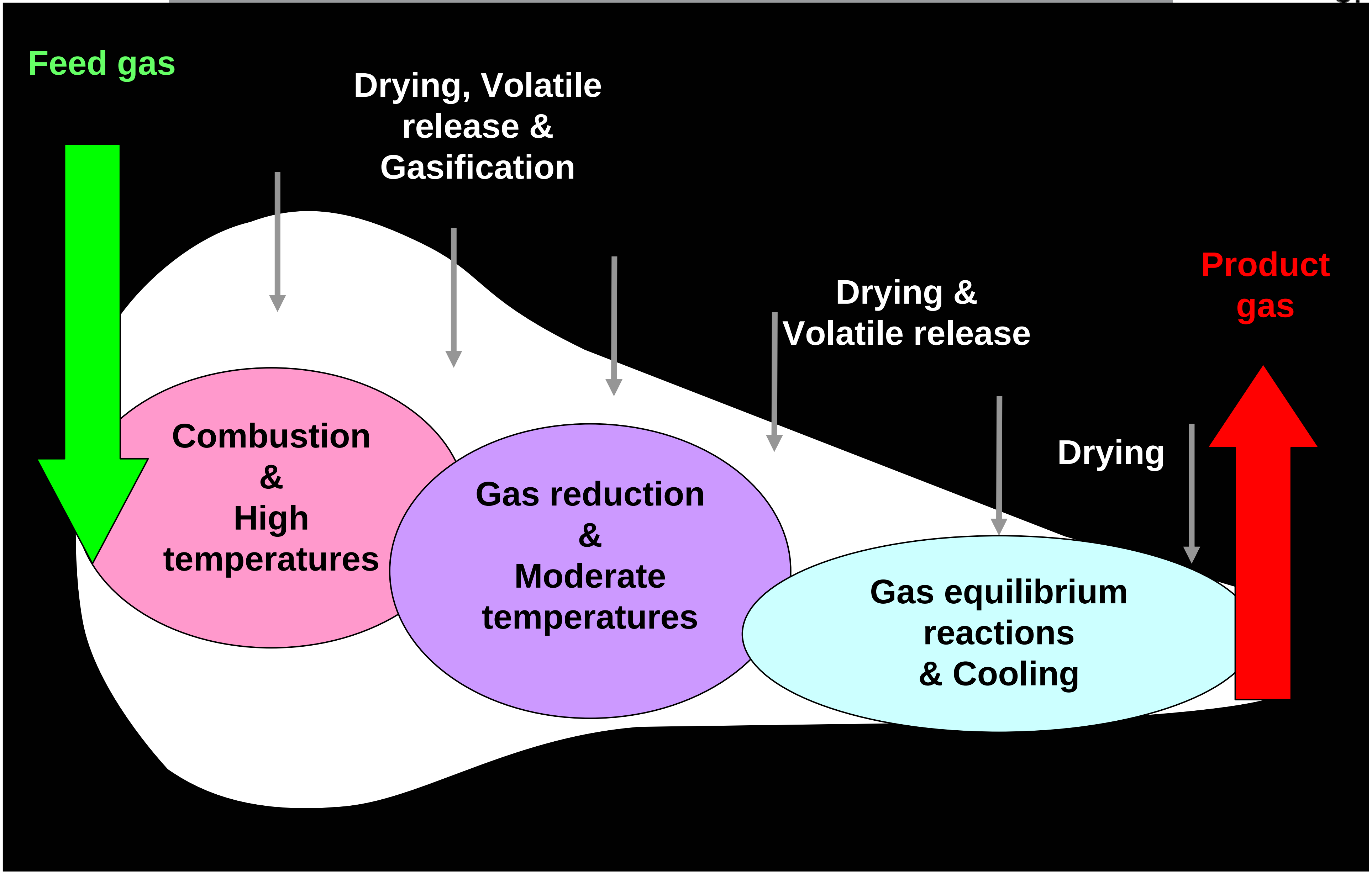
Kolkata, India

Modelling of UCG processes

- ❖**UCG research involves analysis of a complex system of interacting:**
  - Geological factors
  - Gasification process
  - Surface and groundwater impacts
  - Public perceptions
- ❖**Most published models are limited to an analysis of only a part of the process.**
- ❖**This presentation also will be limited to modelling the cavity growth through reaction processes, but a companion presentation discusses modelling of the physical site changes.**

Reaction Processes



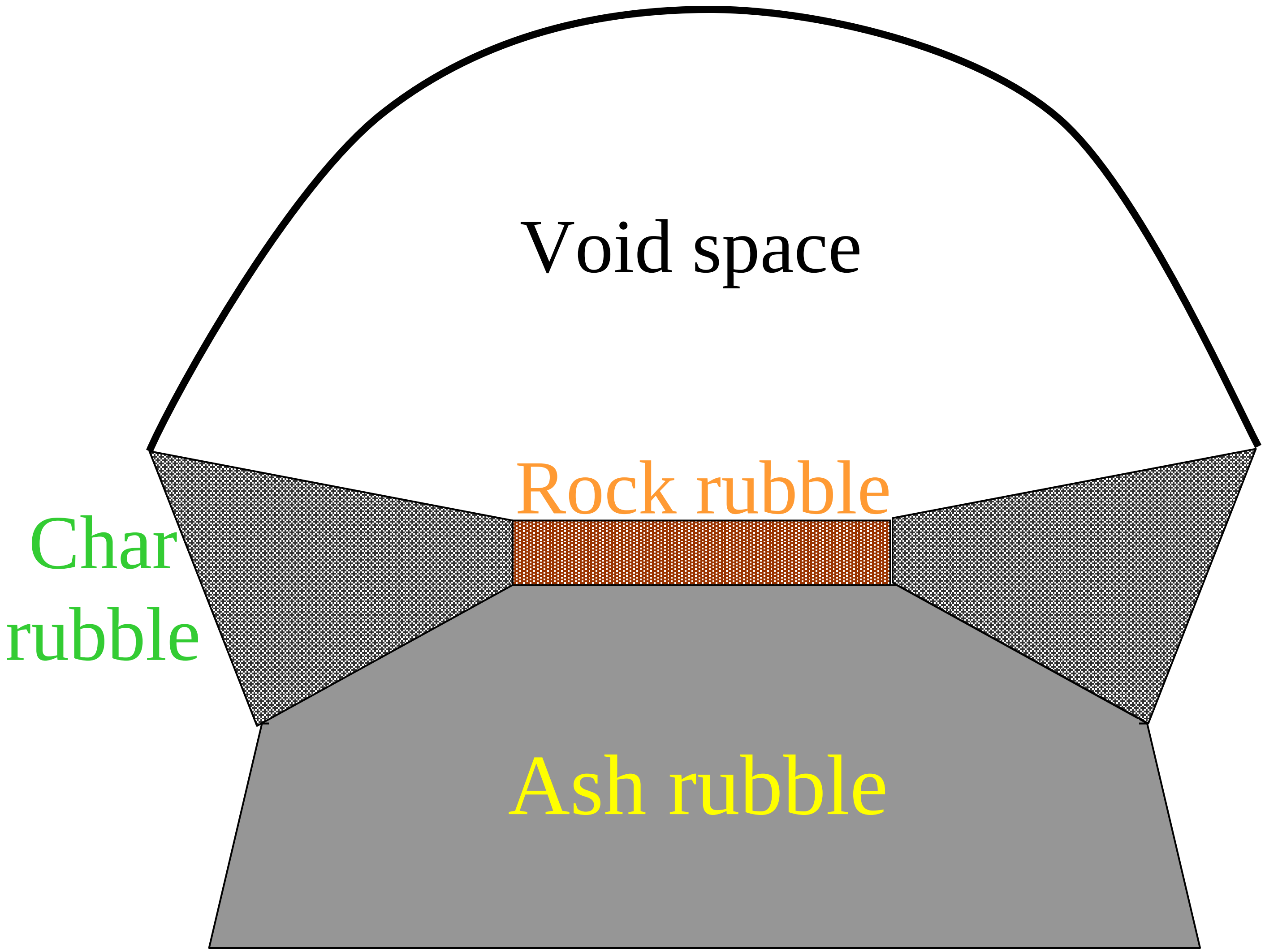
Literature models

- **Selected published models**
  - CAVSIM (Lawrence Livermore)
  - CFD (Delft Univ. of Technology)
  - Box (European Community)
- **Numerous 1-dimensional models have been published with relatively minor differences**

CAVSIM-Lawrence Livermore

- Assumes the gasification cavity will be axisymmetrical around a vertical axis
- Developed to model CRIP experiments performed in the USA
- Limited reaction set, heat transfer and gas flow
- Cavity growth is by ‘spalling’, where material falls off the roof and walls

CAVSIM geometry



CAVSIM summary

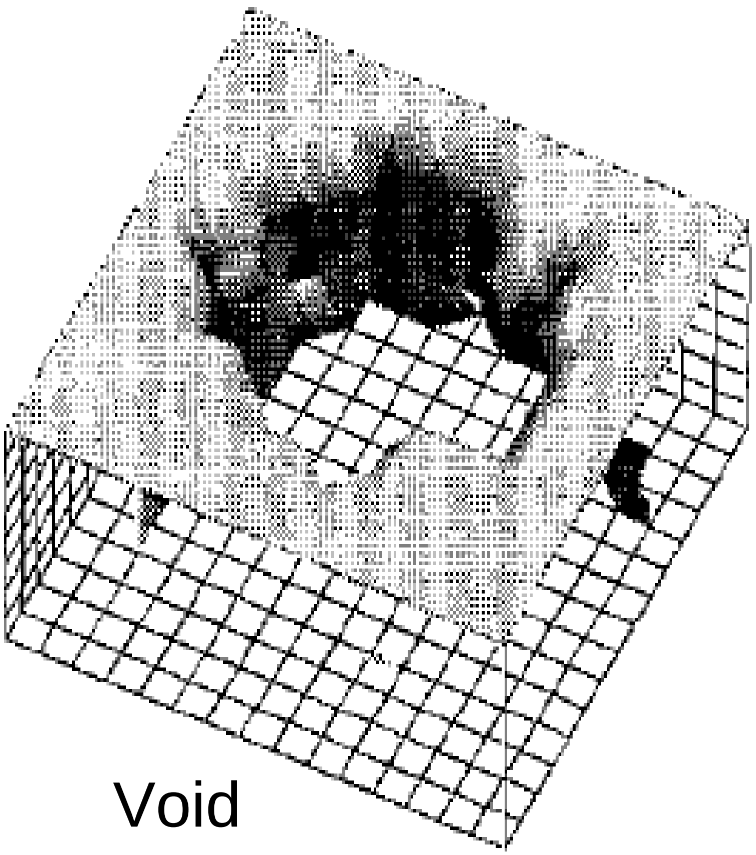
CAVSIM was used successfully to model specific experiments, but was hindered by the difficulty in estimating the ‘spalling’ rate until after the experiment was performed and required corrections when the geometry was disturbed by shortening of the CRIP

CFD-Delft Univ. of Technology

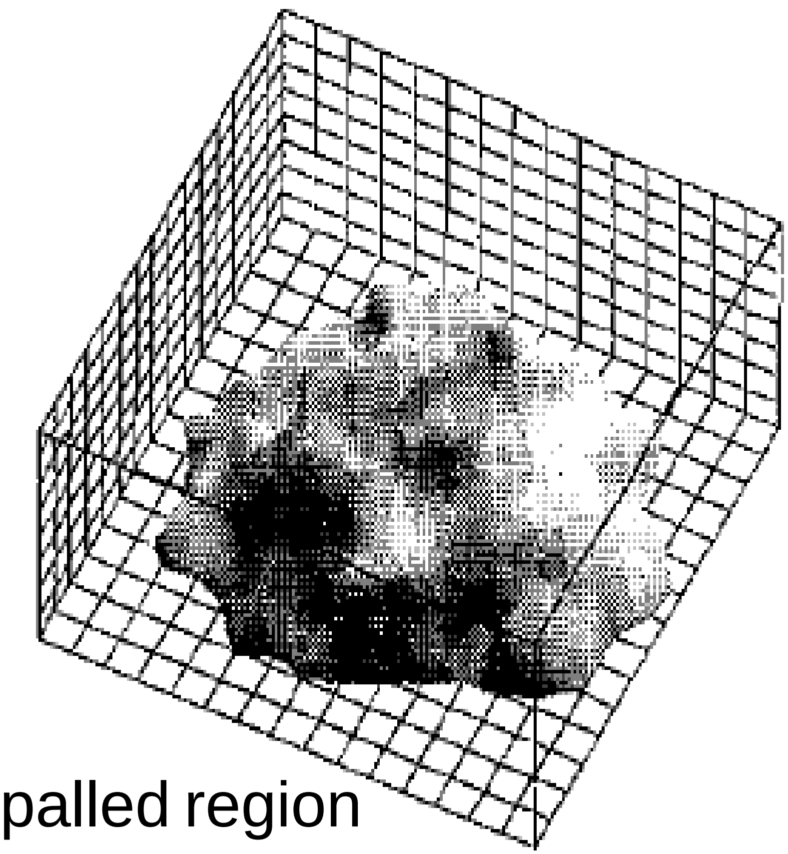
- Series of models developed for the European Community gasification trials
- Considered the site as being composed of numerous finite elements of coal that increased in porosity with reaction
- Simplifying assumptions include constant block temperature and pre-defined gas flow path, but vary between model versions

Delft example

Biezen (1996) produced a model which allowed collapse of material when the porosity becomes excessive. Some factors require fitting to experimental data. The example shown below is based on the Rocky Mountain 1 trial.



Void



Ash/Spalled region

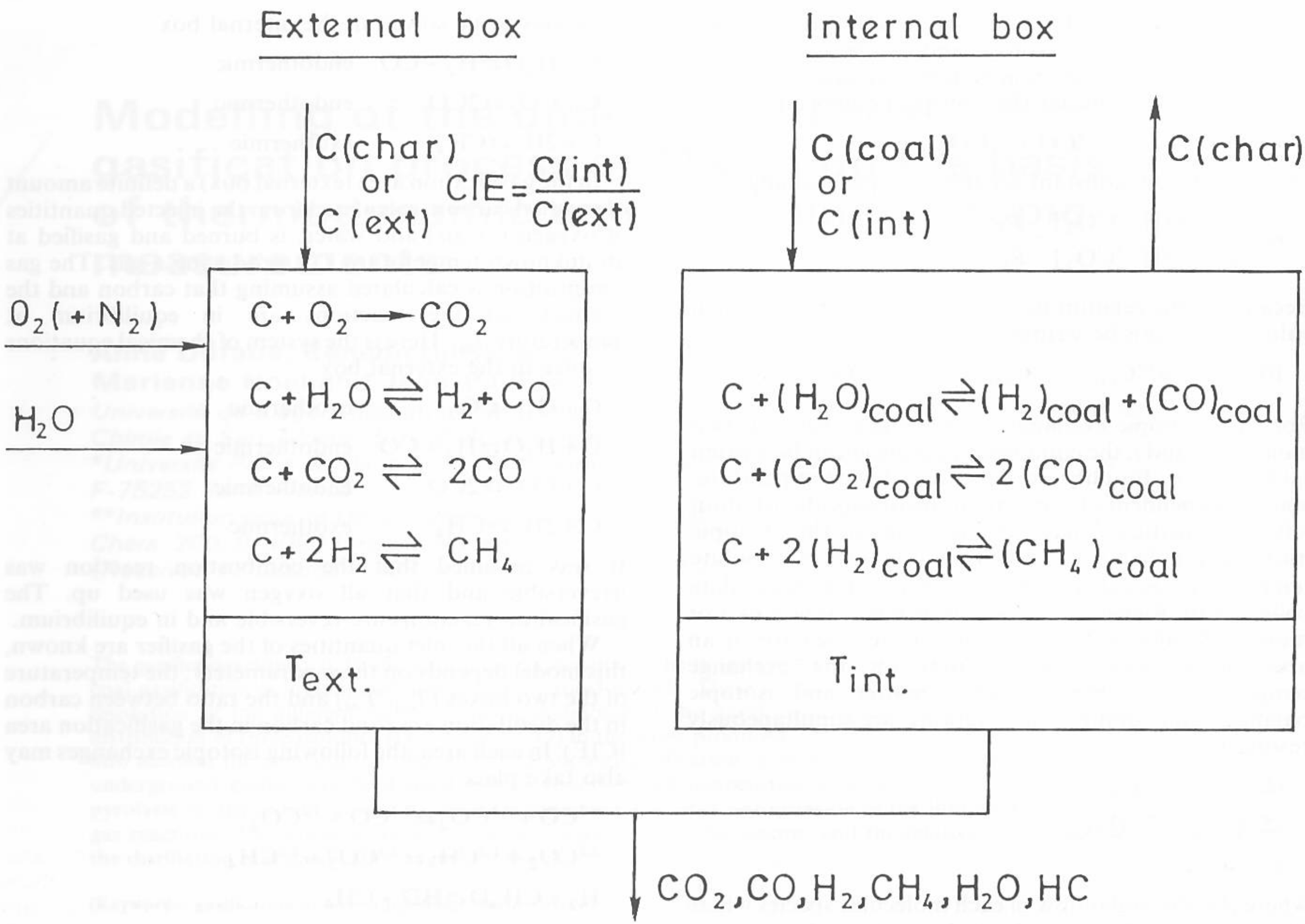
Delft summary

The Delft approach is extremely numerically intensive. Several different models have been published, but they all require simplifying assumptions to allow solutions to be achieved. For example, an average temperature may be used for all coal in the region of the void.

Box models-European Comm.

- **Simplified models that involve zones with pre-defined roles, for example:**
    - First box is a combustion zone
    - Second box has other gasification reactions
    - Third box allows gas bypass of reactions
- **Generally, the product gas is assumed to be at equilibrium at an assumed exit temperature**

2-Box model (Dufaux, 1990)



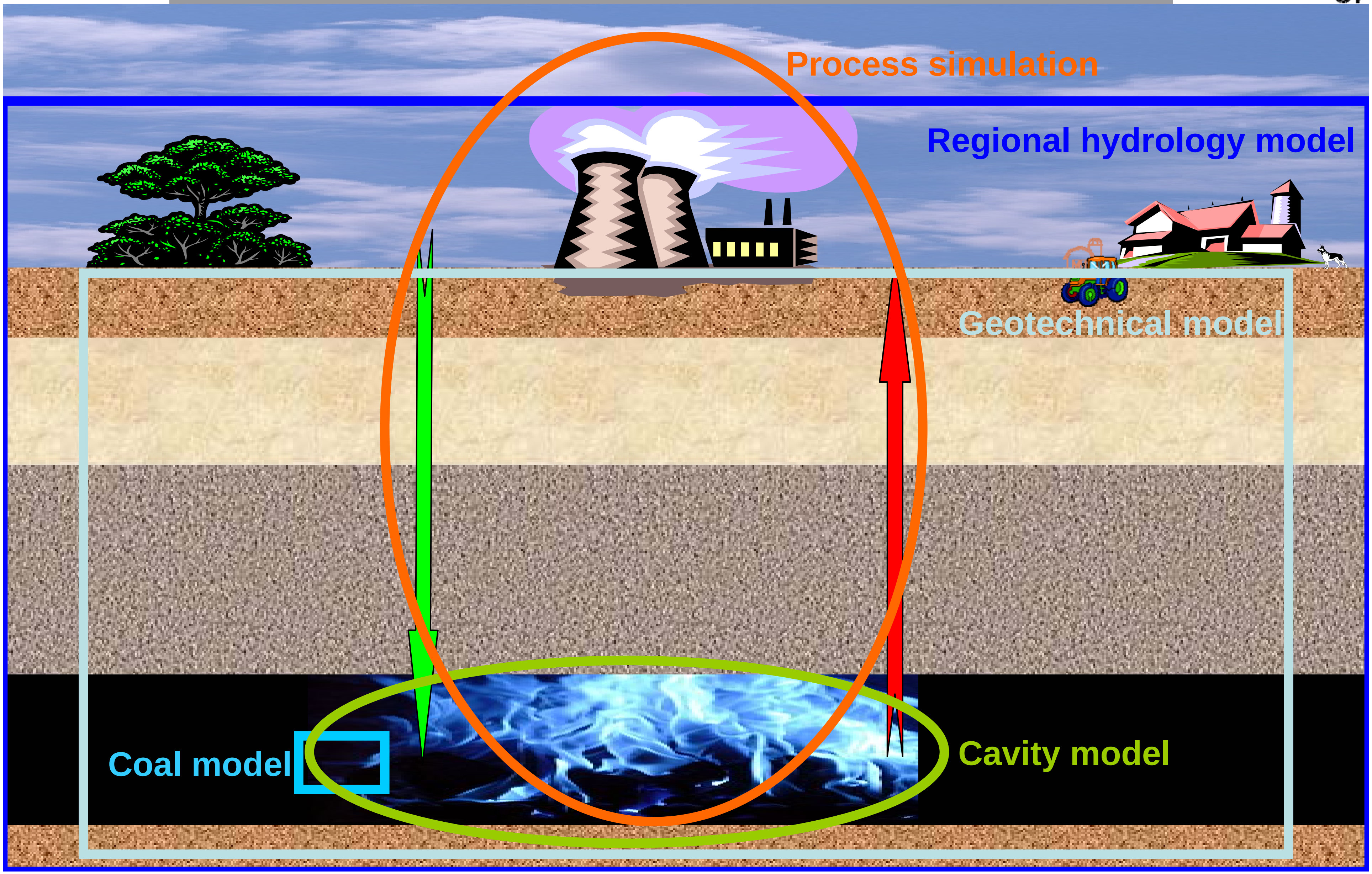
Box model comments

- ❖**This type of modified equilibrium model is useful for rapid predictions**
- ❖**Definition of the boxes is fairly arbitrary and can vary with gasification technique and site characteristics**
- ❖**There is a tendency to increase the number of boxes to improve alignment with experimental results, but this makes it more a correlation than a model**

CSIRO modelling

We have taken a more comprehensive approach to UCG, considering not only the gasification process but also the geotechnical and hydrology interactions. This requires a suite of models, rather than a single model.

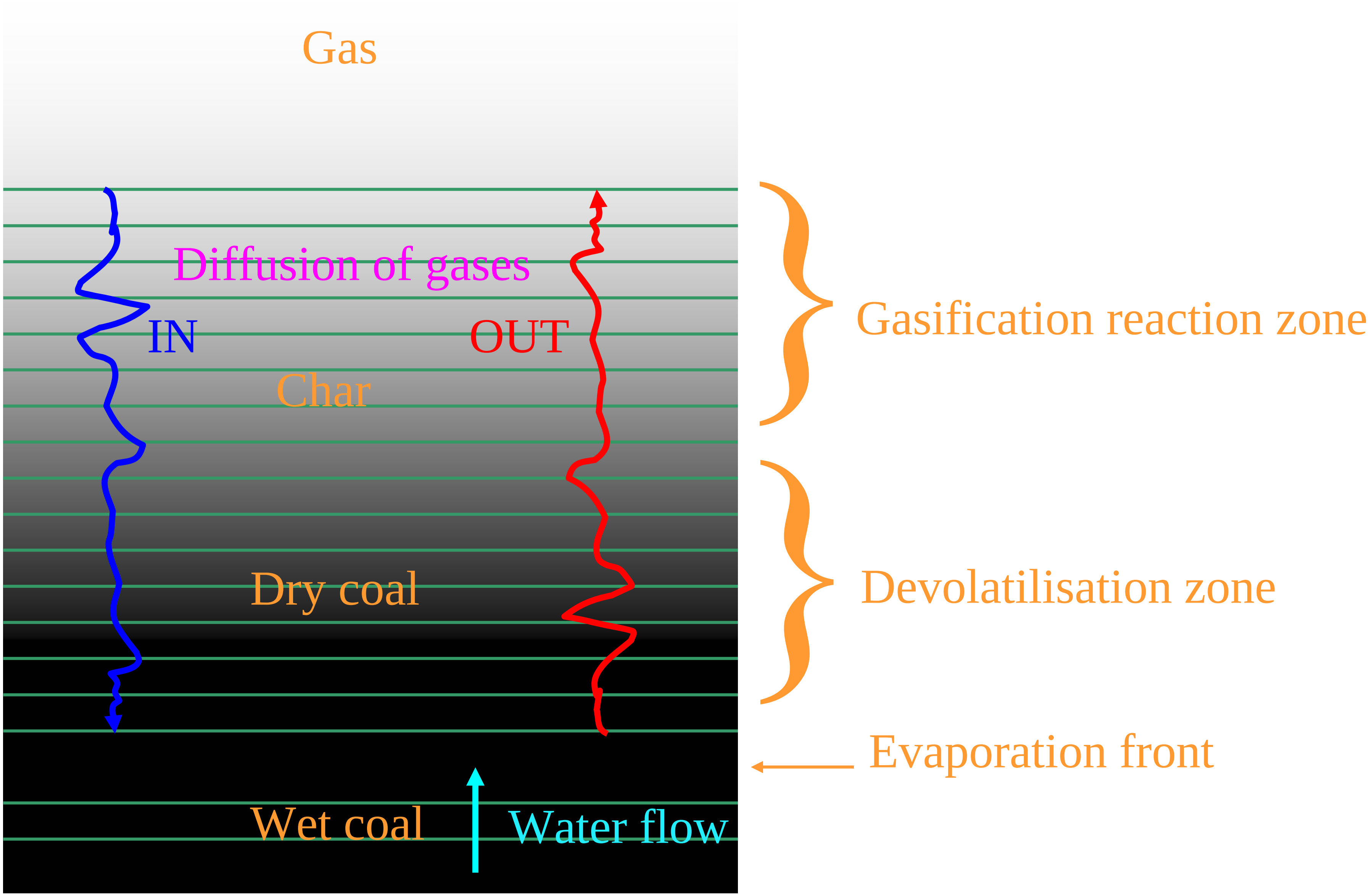
Modelling suite for UCG



Elements of the Coal & Cavity models for UCG

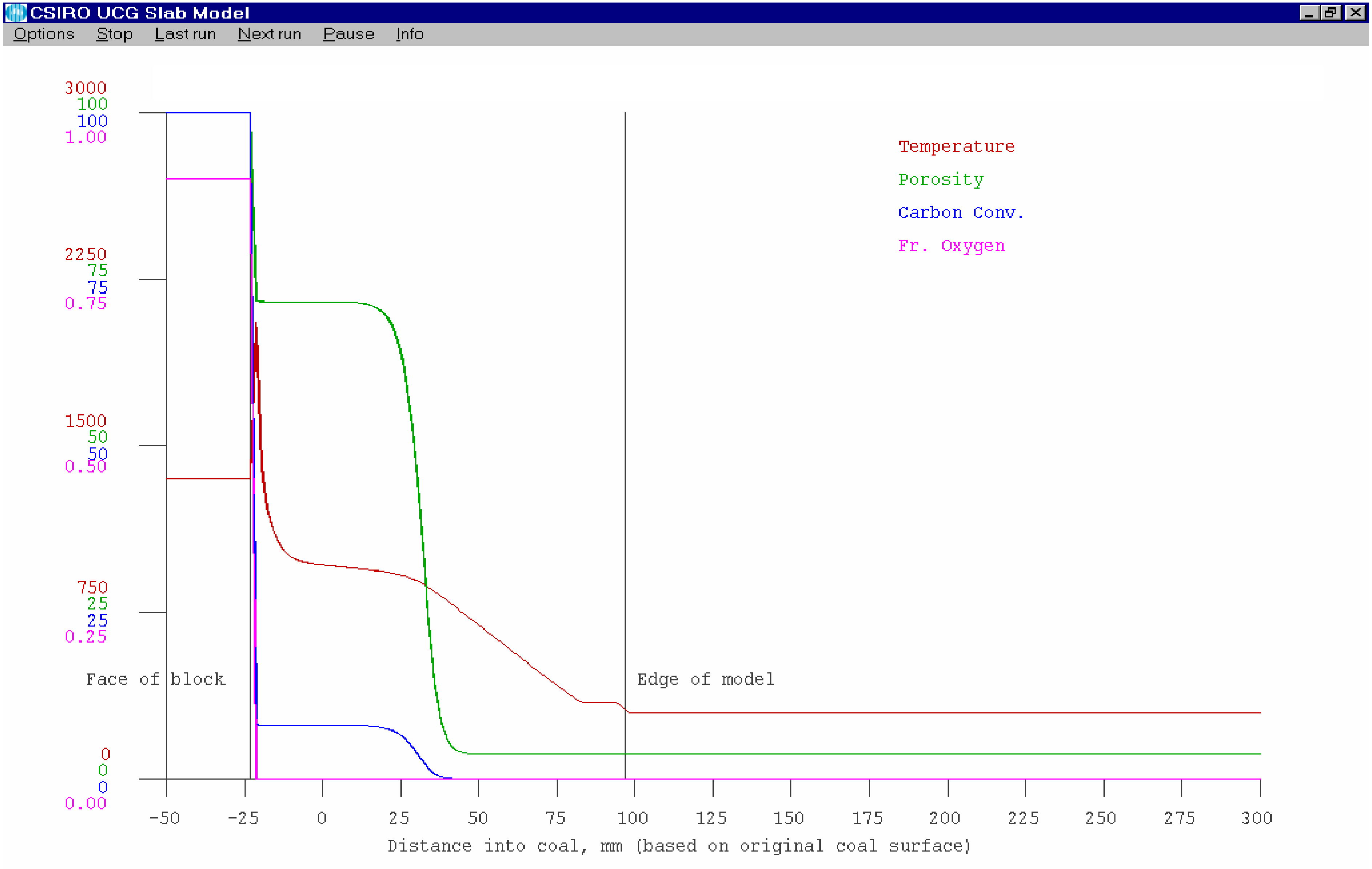
- **Coal & char reactions**
- **Coal/char structural changes**
- **Gas flow and reactions**
- **Water flows and evaporation**
- **Heat transfer**
  - Conduction, convection & radiation
- **Rock & coal breakage and collapse**
- **Resizing of the matrix with growth**

Coal model

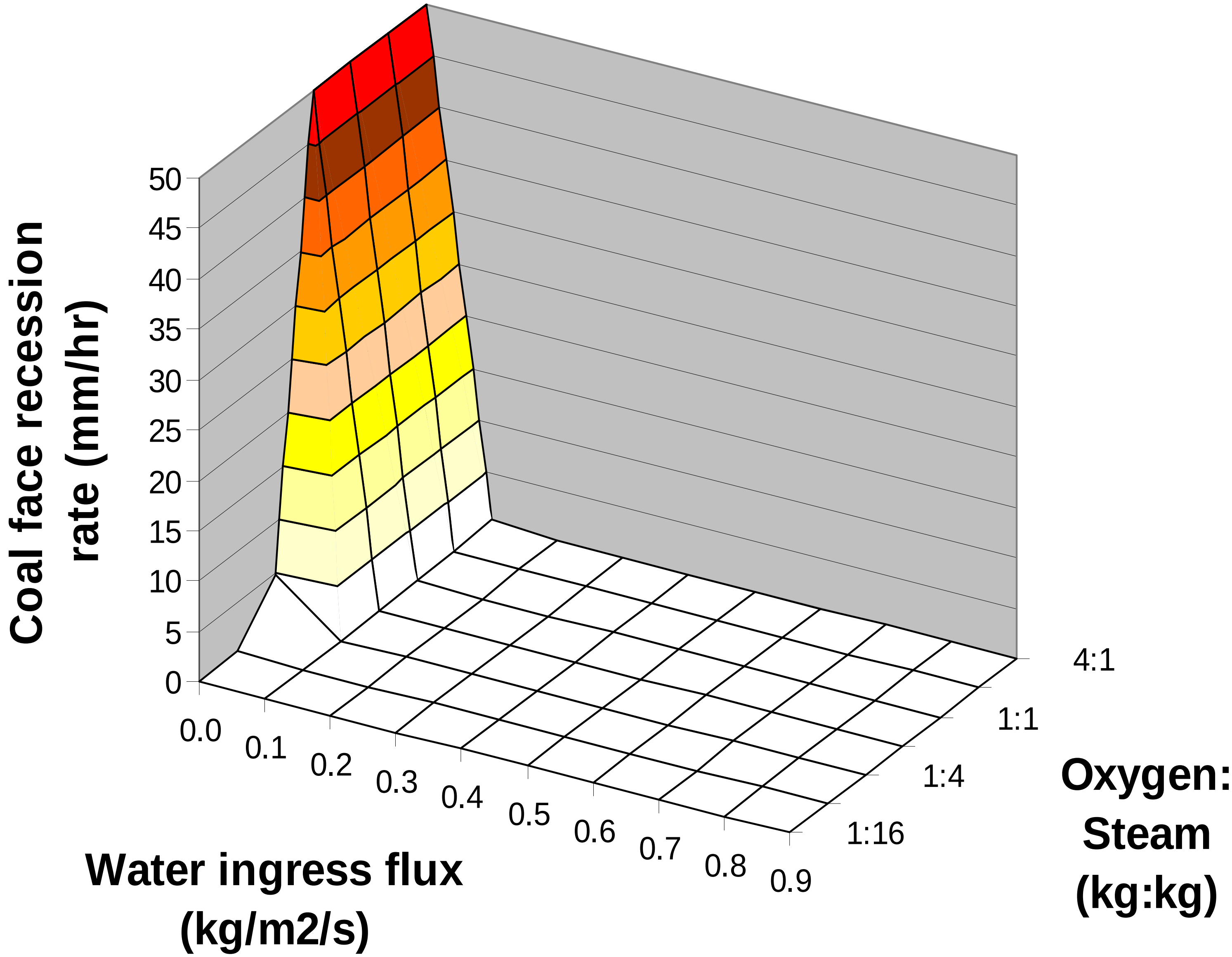


Gas
Diffusion of gases
IN
OUT
Char
Dry coal
Wet coal
Water flow
Gasification reaction zone
Devolatilisation zone
Evaporation front

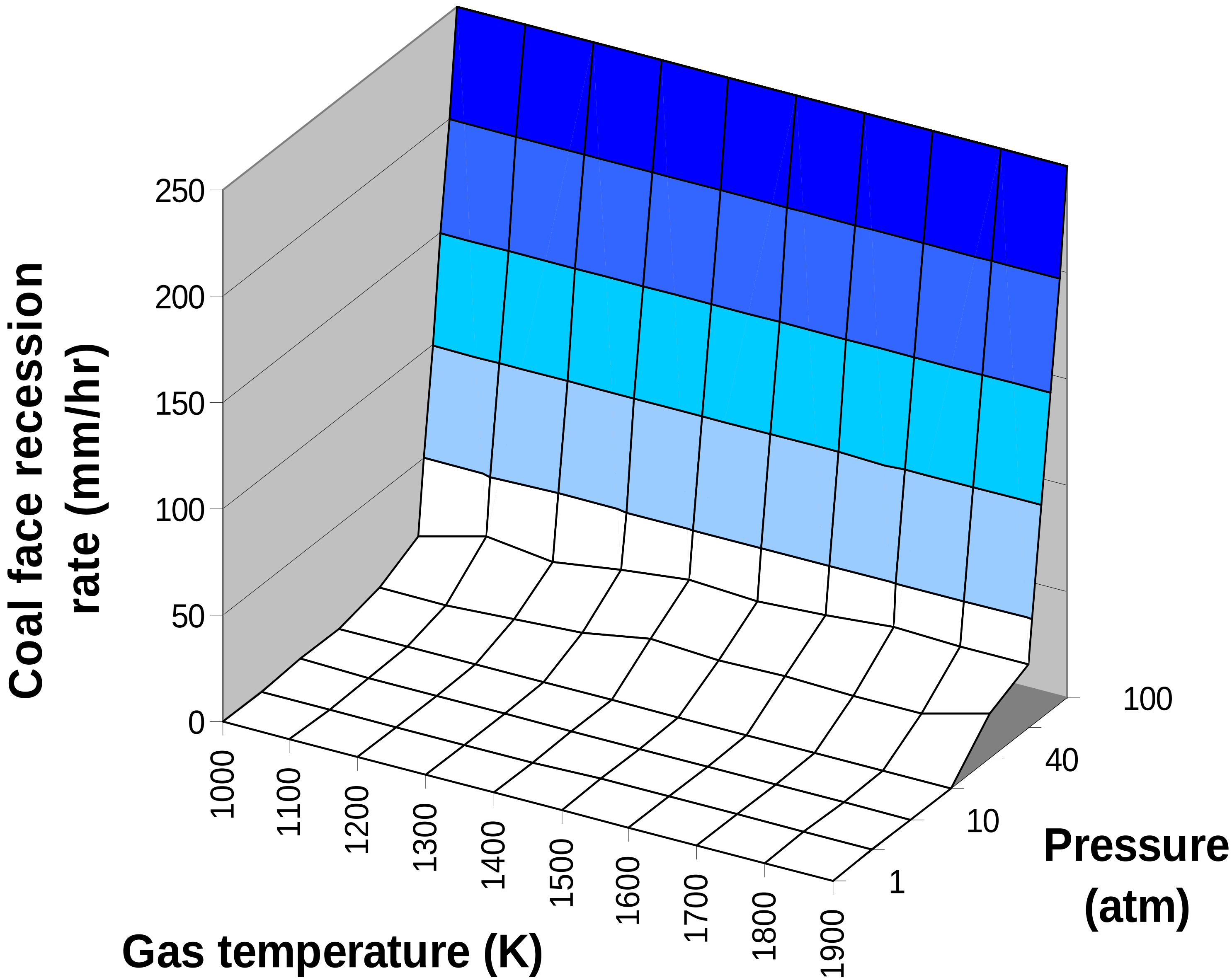
Output from coal model



Predictions from the coal model -Impact of reactant gas mix and water



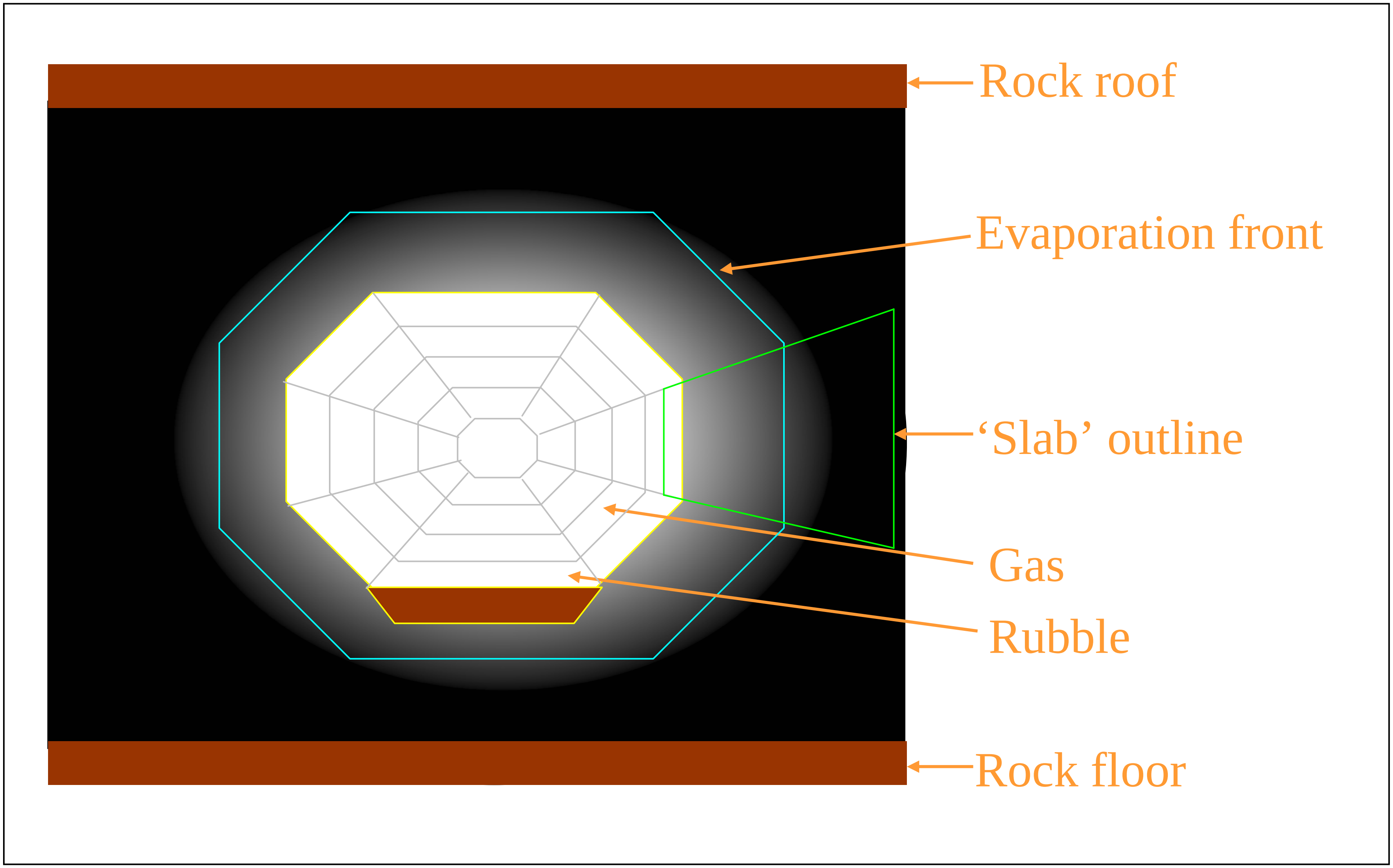
Predictions from the coal model -Impact of pressure and temperature



Use of the coal model

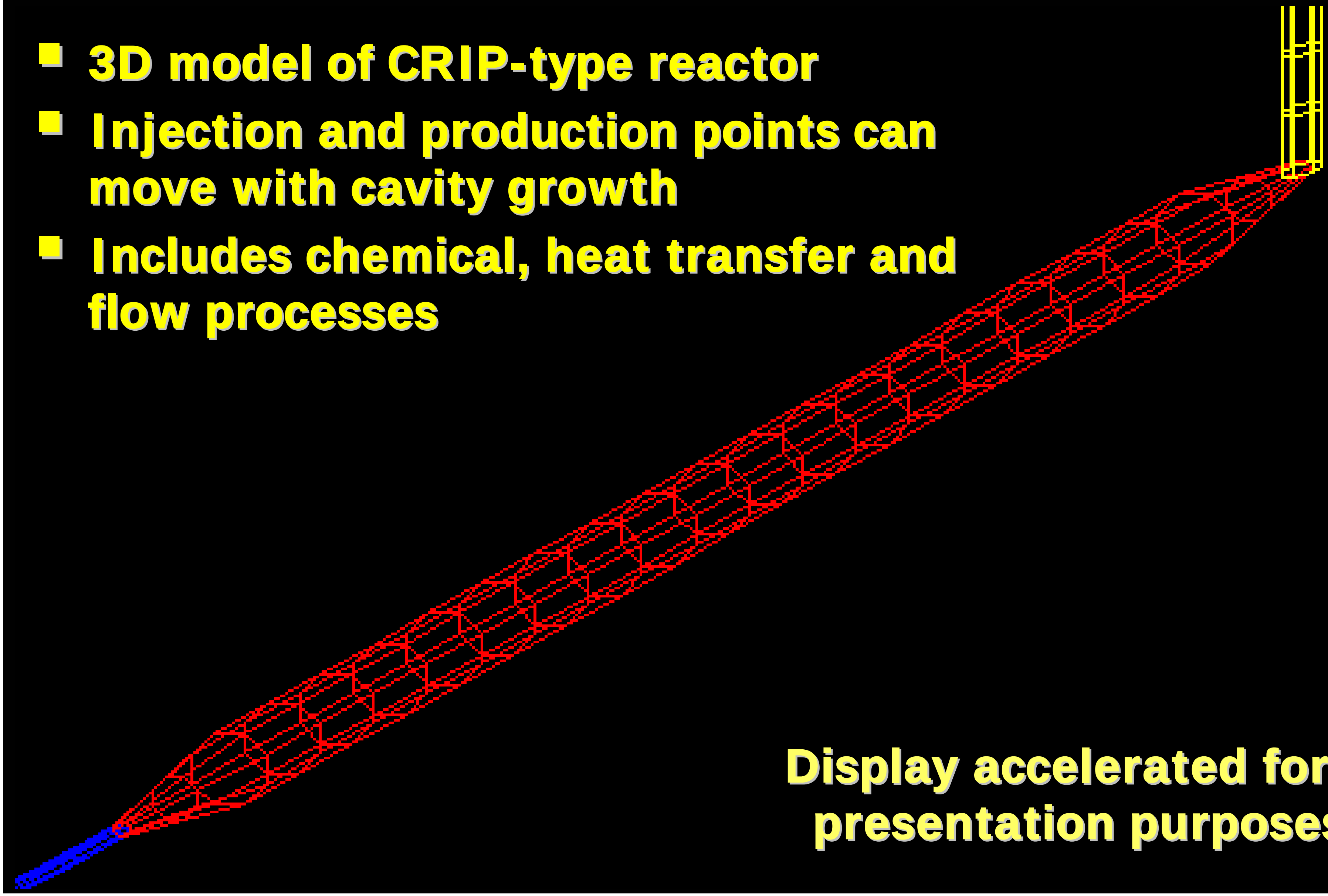
- ❖Does not provide standalone predictions relevant to UCG as it neglects many of the gas flow and heat transfer features of real cavities
- ❖Makes spot predictions of coal behaviour under pseudo-steady state conditions to feed into more complex models
- ❖Can be used to predict the general operating regimes that are desirable for efficient gasification

Cavity model



Cavity model operation

- 3D model of CRIP-type reactor
- Injection and production points can move with cavity growth
- Includes chemical, heat transfer and flow processes



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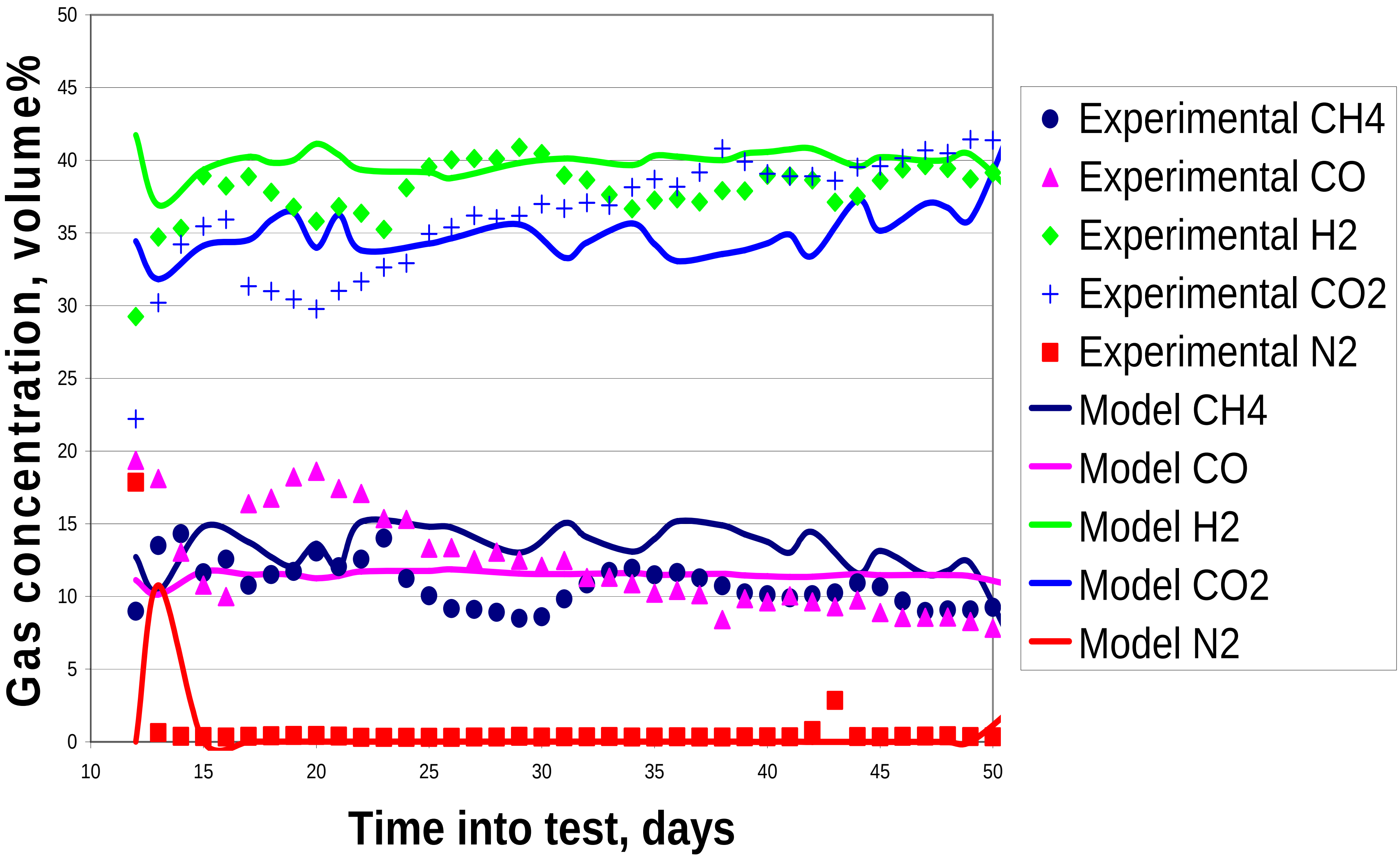
Cavity Model verification versus Rocky Mountain 1 trial 1987-88



Model performance

Predicts accurately:

- Cavity volume changes
- Product gas composition and flow

Hindrances to model performance:

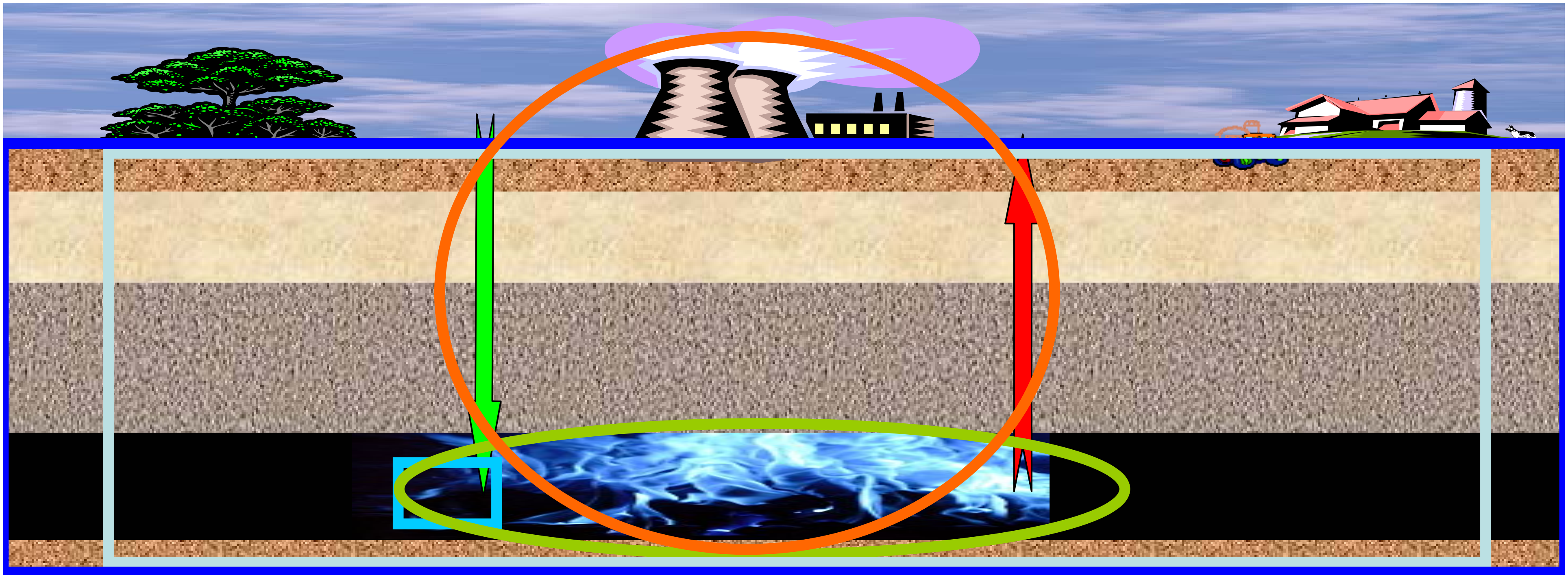
- Requires detailed site information
- Experimentally, the cavity shape was affected by uncontrolled shortening of the ‘CRIP’ and an undetected fault running through the site

Other models

- ❖Geotechnical - COSFLOW is a CSIRO developed model for rock collapse, water flow, contaminant flow and gas flow in mining affected strata.
- ❖Regional hydrology – MODFLOW is a public domain modelling platform for large scale hydrological simulation.
- ❖Process simulation – HYSYS.Process is commercial software package that can be used to simulate power production and chemical production from UCG product gas.

Summary

There have been numerous published models relating to UCG, however, it is apparent that the interaction of the underground reactions with the geological 'container' requires a more comprehensive approach that includes the



The End

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- Austr