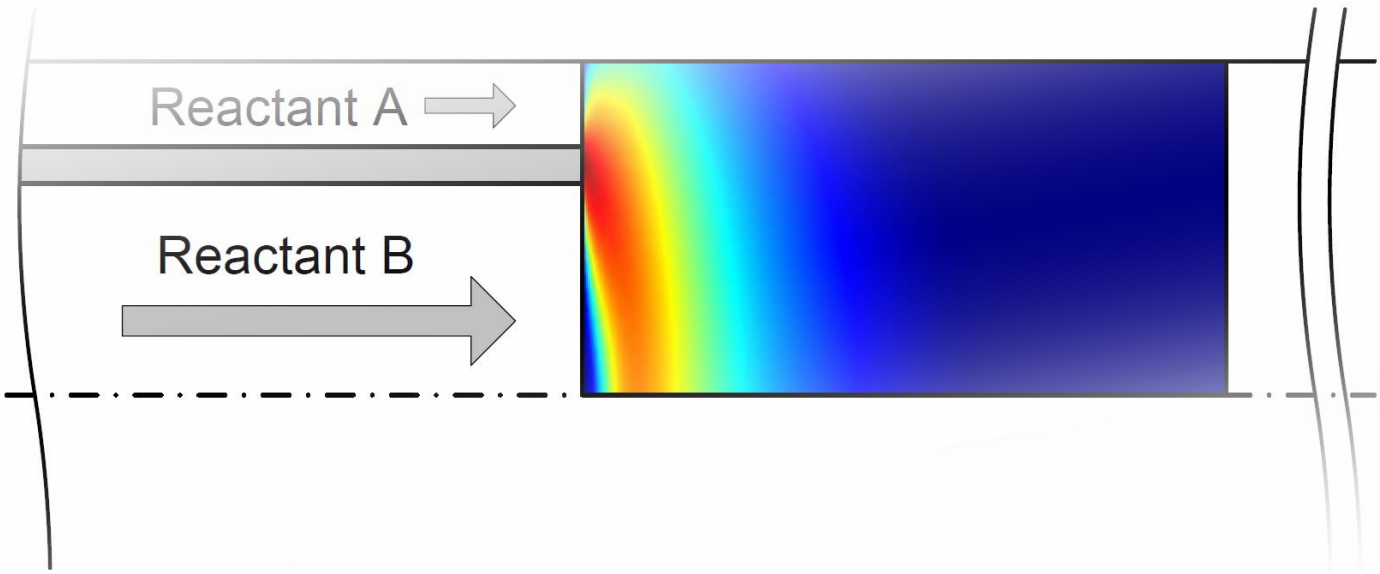
user story

probability density function methods for turbulent reacting flows

solutions for off-the-shelf CFD codes



CFD methods typically solve for average quantities, for example species concentration and temperature. Turbulent reacting flow models must approximate the rates of species formation and energy release based on these average quantities. This is often a poor approximation.

THE CHALLENGE

Turbulent reaction modelling in 3D CFD

THE SOLUTION

Combine a conventional CFD code with efficient implementations of two recent probability density function-based reaction models

THE RESULTS

- A new product: dqmomsf
- Suitable for convetional CFD codes
- Applicable to all flows and all chemistry

Existing models used for CFD calculations of turbulent reacting flow are normally make strong assumptions about the chemistry or the flow. For example, that the chemistry is very fast and the reaction is controlled by the rate of turbulent mixing. and the flow. This type of assumption is not suitable for many important slower reactions, such as those responsible for describing the formation of NOx and soot in a diesel engine.

THE CHALLENGE

The most general approach to turbulent reaction models are probability density function methods. These make no assumptions about either the chemistry or the flow and are widely used by the combustion research community. However, existing solution methods are computationally expensive and are not amenable to conventional CFD. The challenge was to combine the benefits of the probability density function approach with standard CFD methods. The objective was to develop a fast and generally applicable method that could be used as an add-on to off-the-shelf CFD codes to enable complex turbulent reaction chemistry to be combined with the 3D modelling capability of the CFD.

THE SOLUTION

Efficient and robust algorithms were developed for two recent probability density function methods. The implementation enables the model to be used as an add-on with conventional CFD codes.

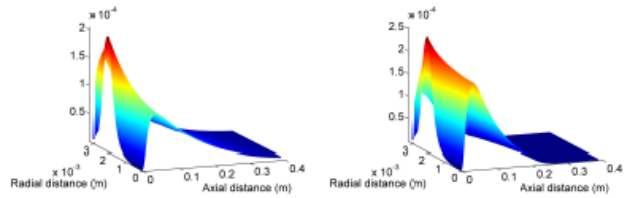
The capabilities of the model were assessed against a known test case.

cmcl innovations

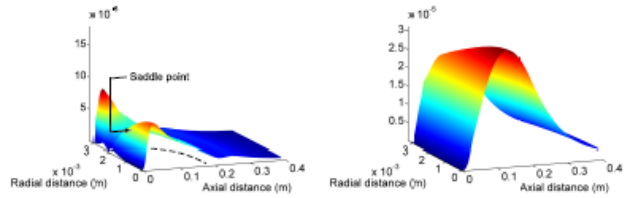
e-mail: enquiries@cmclinnovations.com **web:** www.cmclinnovations.com

user story

$$A + B \xrightarrow{k_1} R,\ B + R \xrightarrow{k_2} S$$



(a) *Empirical standard deviation, species A.* (b) *Empirical standard deviation, species B.*



(c) *Empirical standard deviation, species R.* (d) *Empirical standard deviation, species S.*

Spatial distribution of sub-grid segregation of chemical species for the test reaction. This information is critical for the accurate prediction of the test reaction yield.

DQMoM-IEM yield (%)			Literature yield data (%)	
$N=2$ [a]	$N=2$ [b]	$N=3$ [b]	Transported PDF [c]	Expt. [d]
80.4	80.7	81.9	81.0	82.1

[a] *Analytic solver* [b] *General solver* [c] *Tsai and Fox [Table 3]* [d] *Li and Toor [Table 1]*

DQMoM-IEM yields versus test case data.

Tsai and Fox (1994), doi:10.1016/0009-2509(94)00270-3
Li and Toor (1986), doi:10.1002/aic.690320809

APPLICATION AREAS

• 3D turbulent reaction simulations post-burn combustion emissions

PRODUCTS USED

• dqmomsf

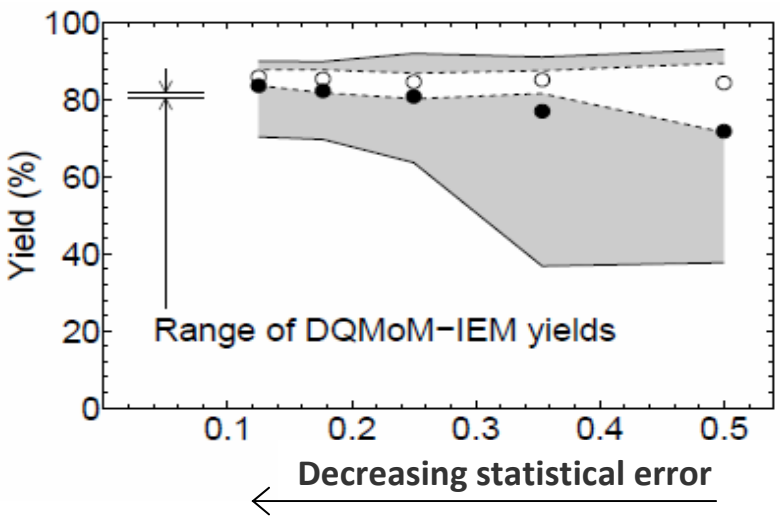
THE RESULTS

• Two general turbulent reaction models for 3D CFD

The SF method uses an efficient Monte Carlo solver. It is suitable for chemitry of arbitrary complexity. Users may refine the level of Monte Carlo approximation to move between quick 'back of the envelope' calculations and more expensive highly detailed calculations.

• Choose the level of detail to suit the problem and the computation budget

The DQMoM-IEM method replaces the SF Monte Carlo solver with a deterministic method. Users may refine the level of approximation as required without incurring any statistical error. This provides the option of very fast calculations with results that are far batter than just 'back of the envelope'. See the figures to the left.



This diagram shows the predicted test reaction yields (vertical axis) versus the level of approximation in the simulations (horizontal axis). The circles represent time-avergaed yields calculated using the SF method. The solid circles are for a standard Monte Carlo method, the hollow circles for the cmcl solver. The shaded areas represent the uncertainty due to statistical errors in the SF data. The grey area is for the standard Monte Carlo solver, the white area in the middle is for the cmcl solver. The cmcl xolver provides a more consisent estimate of the yield with much reduced uncertainty. In this example, the DQMoM-IEM method provides comparable estimates in a fraction of the computational time.

cmcl innovations

e-mail: enquiries@cmclinnovations.com **web:** www.cmclinnovations.com