UNIVERSITY OF Southampton

Engineering and the Environment

Aeronautics, Astronautics and Computational Engineering

Simulation of spray combustion for aero-nautical gas turbines

UTC for Computational Engineering

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Challenges in spray modelling

Accurate modelling of the spray evaporation rate is a key requirement for prediction of spray combustion in aeronautical combustors. The location of spray evaporation affects the amount of pollutants produced and the temperature distribution at the combustor exit. The evaporation rate of each droplet depends on the temperature, velocity and composition of the surrounding gas, but each of these 'seen' gas-phase properties fluctuates due to turbulence. Current CFD models neglect these turbulent fluctuations. This project has quantified the evaporation rate errors caused by neglecting turbulent fluctuations and, since they can be very significant, we have developed a computationally efficient model which takes them into account.

Modelling framework

- *The evaporation rate of a fuel droplet depends on the its diameter, temperature and velocity, but also the 'seen' composition, temperature and velocity in the surrounding gas.*

$$\dot{S} = fn(\underbrace{T_{seen}, Y^{fuel}_{seen}, u_{seen}}_{\text{seen quantities}}, \underbrace{d_{droplet}, T_{droplet}, u_{droplet}}_{\text{droplet quantities}})$$

- *CFD simulations for a combustor rely on models for the mean evaporation rate of all the droplets in a computational cell. To compute the mean evaporation rate we need to estimate the joint-probability (PDF) of all the inputs to the droplet evaporation rate model.*
- *Several approaches are available to estimate the joint-PDF of seen droplet properties:*

1. *Solve PDF equations for the seen properties – this is prohibitively expensive.*
2. *Neglect all turbulent fluctuations of T_{seen} and Y_{seen} – this is standard practice.*
3. *Presume the PDF of each seen property and assume independence – this is a recent improvement presented by Bilger [1], and De [2]:*

$$Pr(T_{seen}, Y^{fuel}_{seen}, u_{seen}) = Pr(T_{seen})Pr(Y^{fuel}_{seen})Pr(u_{seen})$$

4. *Presume the joint-PDF of all seen properties – this more accurate method is developed below*

Presumed joint-PDF method

- *The temperature and composition are modelled as a function of mixture fraction Z and progress variable C (the flamelet approach).*
- *The mixture fraction Z and progress variable C pdfs are modelled with presumed beta pdfs.*
- *Correlation between Z and C is captured by use of a Plackett copula.*
- *Seen properties are sampled from the joint Z-C distribution using a new efficient sampling procedure.*
- *Steady state evaporation rate is calculated:* $\frac{dD^2}{dt} = \lambda_{st}$

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[1] Bilger, Combustion and Flame 158.2 (2011): 191-202. [2] De, Kim, Combustion and Flame (2013).

Conclusions

- *Turbulent fluctuations of composition and temperature have a leading order effect on the mean evaporation rate.*
- *In this simple test case, up to 70% difference in evaporation rate was observed between negative and positive Z-C correlations.*
- *This effect is most pronounced for the fuel-lean conditions targeted for gas turbine combustion.*
- *A computationally efficient model for the mean evaporation rate which accounts for turbulent fluctuations and correlations has been demonstrated and is ready for testing in CFD.*

Model performance

- *The Placket Copula produces a presumed joint-PDF which is consistent with the specified marginal PDFs of mixture fraction and progress variable and also accounts for the correlation of mixture fraction and progress variable.*

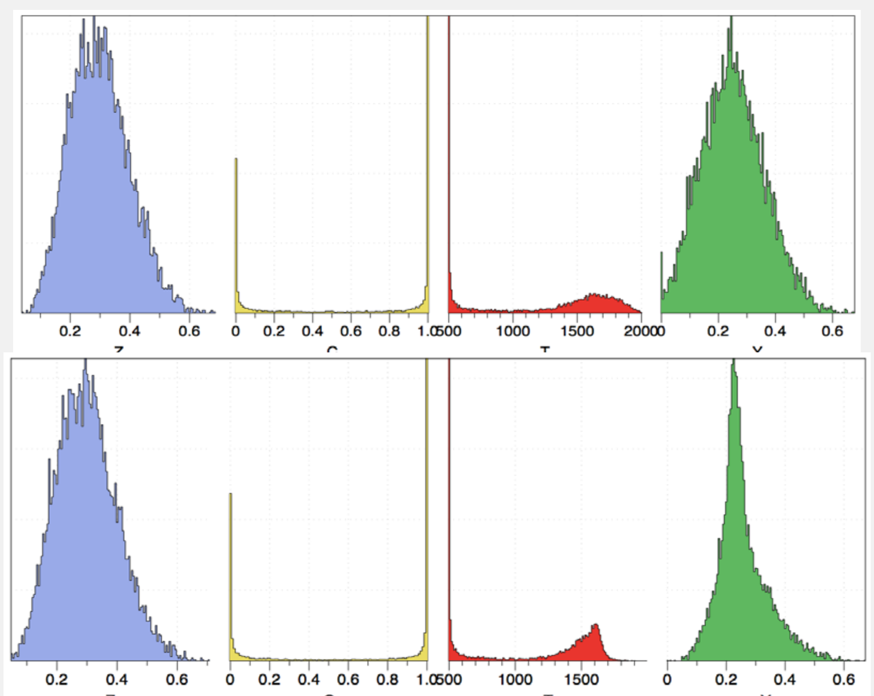

Figure 1: Pdfs for Z (blue), C (yellow), T (red), Y_{fuel} (green) with zero correlation (top) and positive correlation 0.7 (bottom), for <Z>=0.3, Z"²=0.01, <C>=0.6, C"²=0.2.

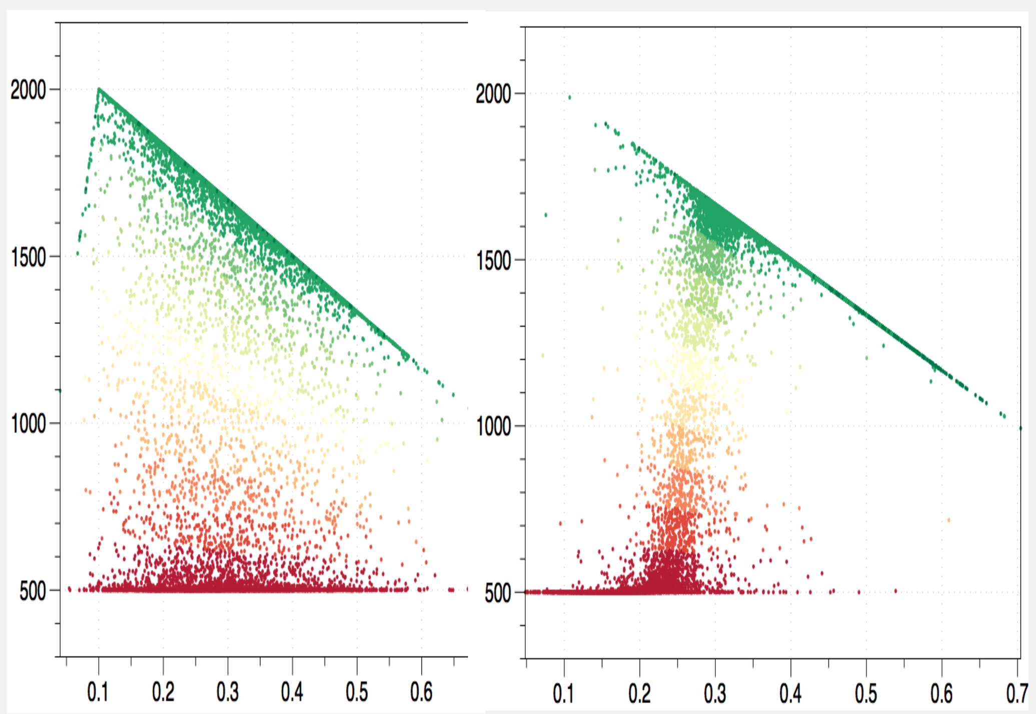

Figure 2: Sampled temperature (K) vs. mixture fraction. Left: zero correlation, Right: positive correlation 0.7.

- *Computing the entire Copula-PDF is costly but for spray modelling we only need a small sample of points – an efficient method for collecting small samples from multivariate Copulas has been developed.*

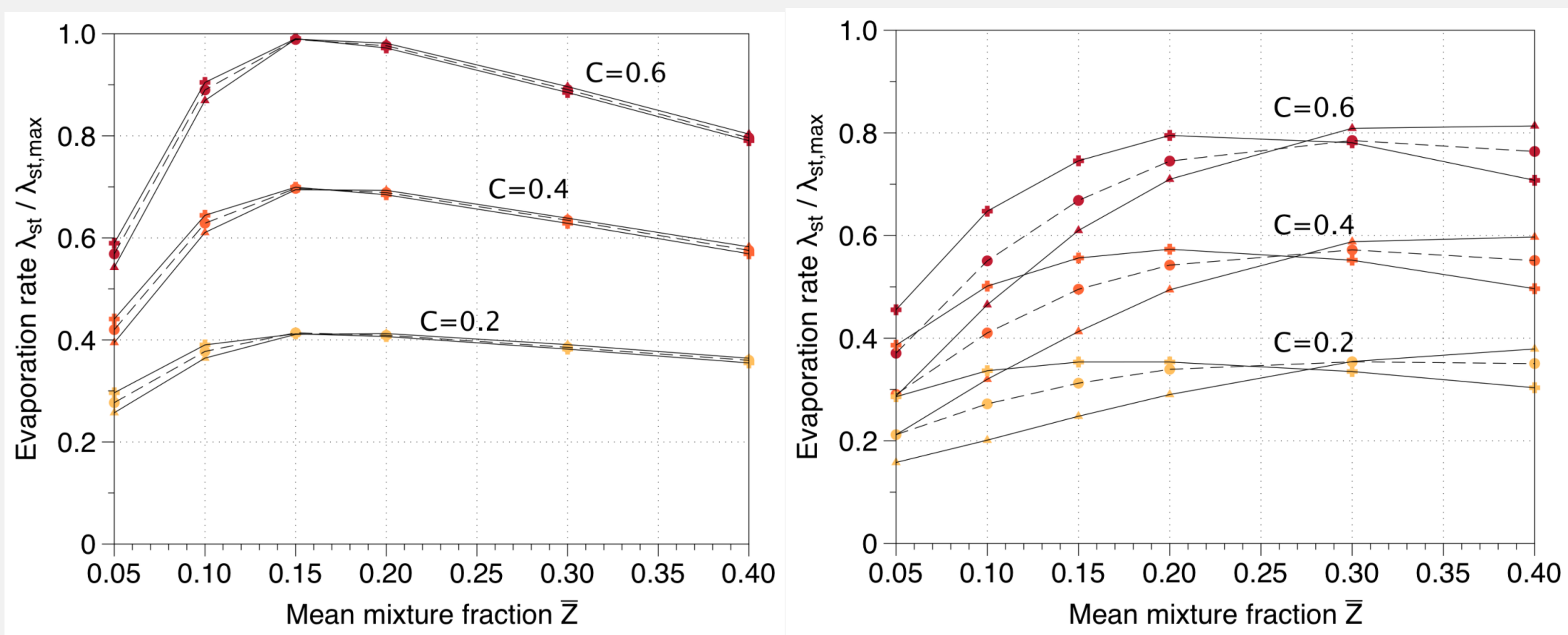

Figure 3: Mean evaporation rate over 10,000 samples against mean mixture fraction. (+) positive correlation 0.7 (o) zero correlation (▲) negative correlation -0.7. Left: C segregation=Z segregation = 0.02; Right: C segregation = Z segregation = 0.2.

- *Figure 3 shows that composition variance has a dramatic leading-order effect on the mean evaporation rate – reducing evaporation rate under lean-burn conditions.*
- *Positive Z-C correlation increases evaporation rates <20% under certain lean-burn conditions (negative correlation leads to a reduction).*

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