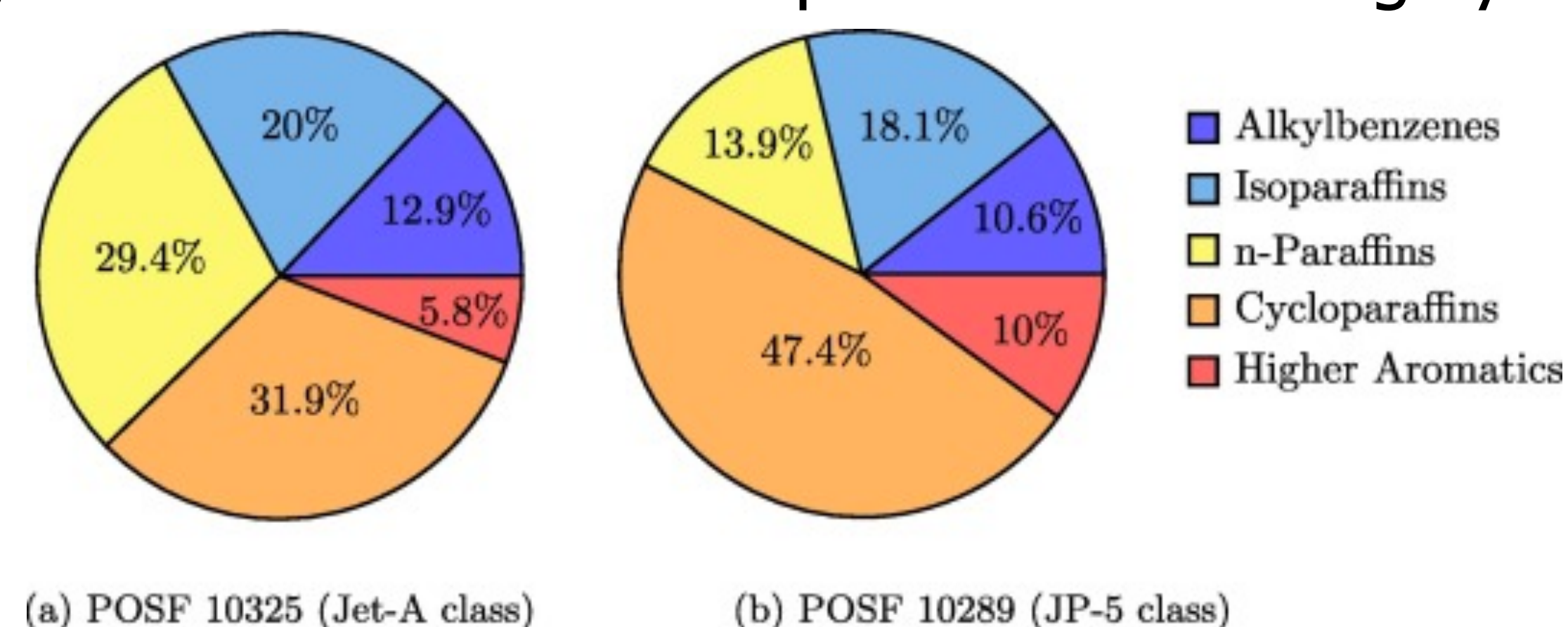


### Motivation and Background

Modern gas turbines are designed to be highly efficient while simultaneously limiting the amount of harmful emissions produced. There is a desire to develop new jet fuels which are renewable and allow for energy independence. However, the performance of these fuels must be carefully considered before use in current or next generation gas turbines.

State-of-the-art multiphysics computer simulations are applied to investigate the behavior of new fuels at conditions near lean blowout, where the combustion process can be highly unstable.



Chemical component distribution of two jet fuels

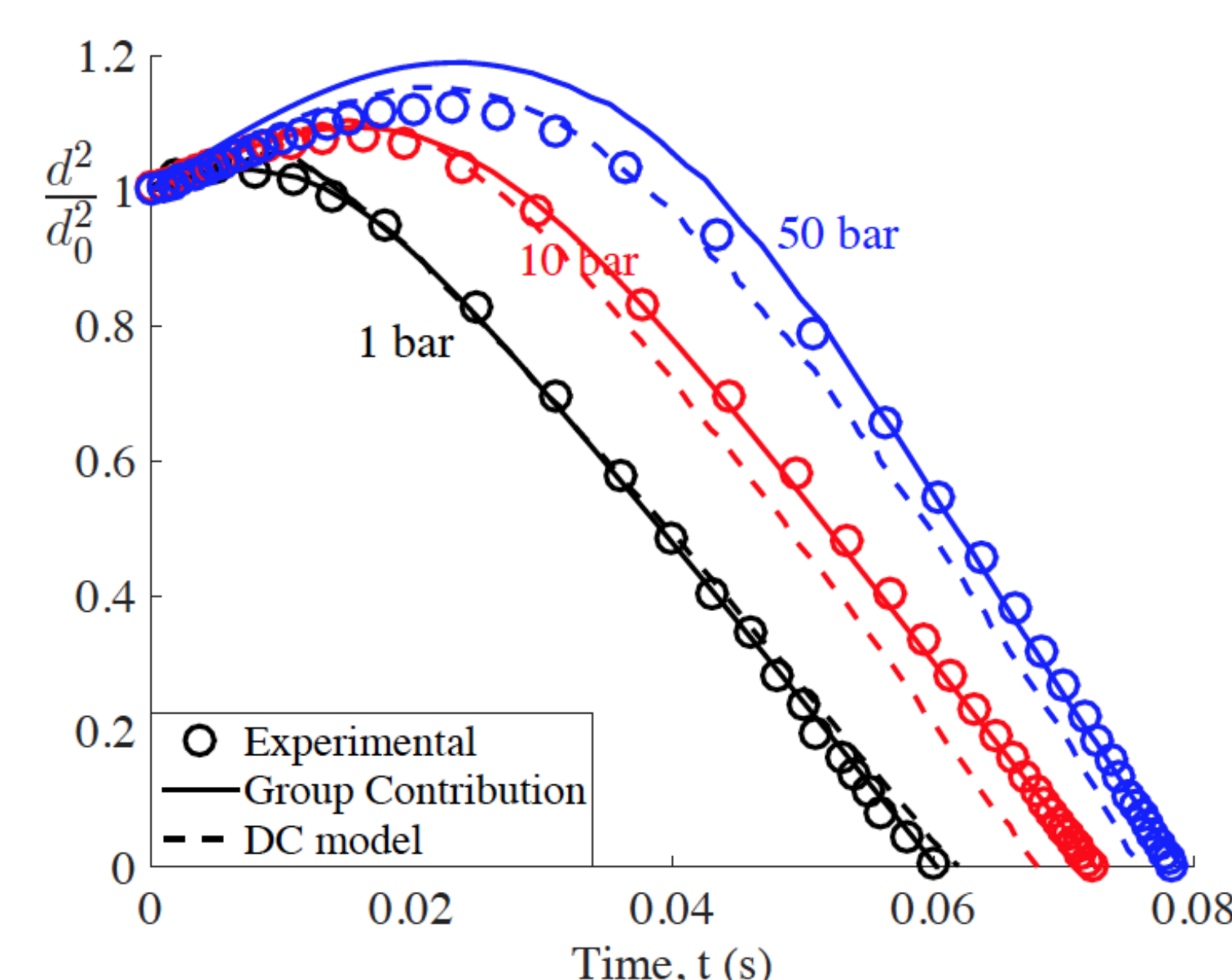
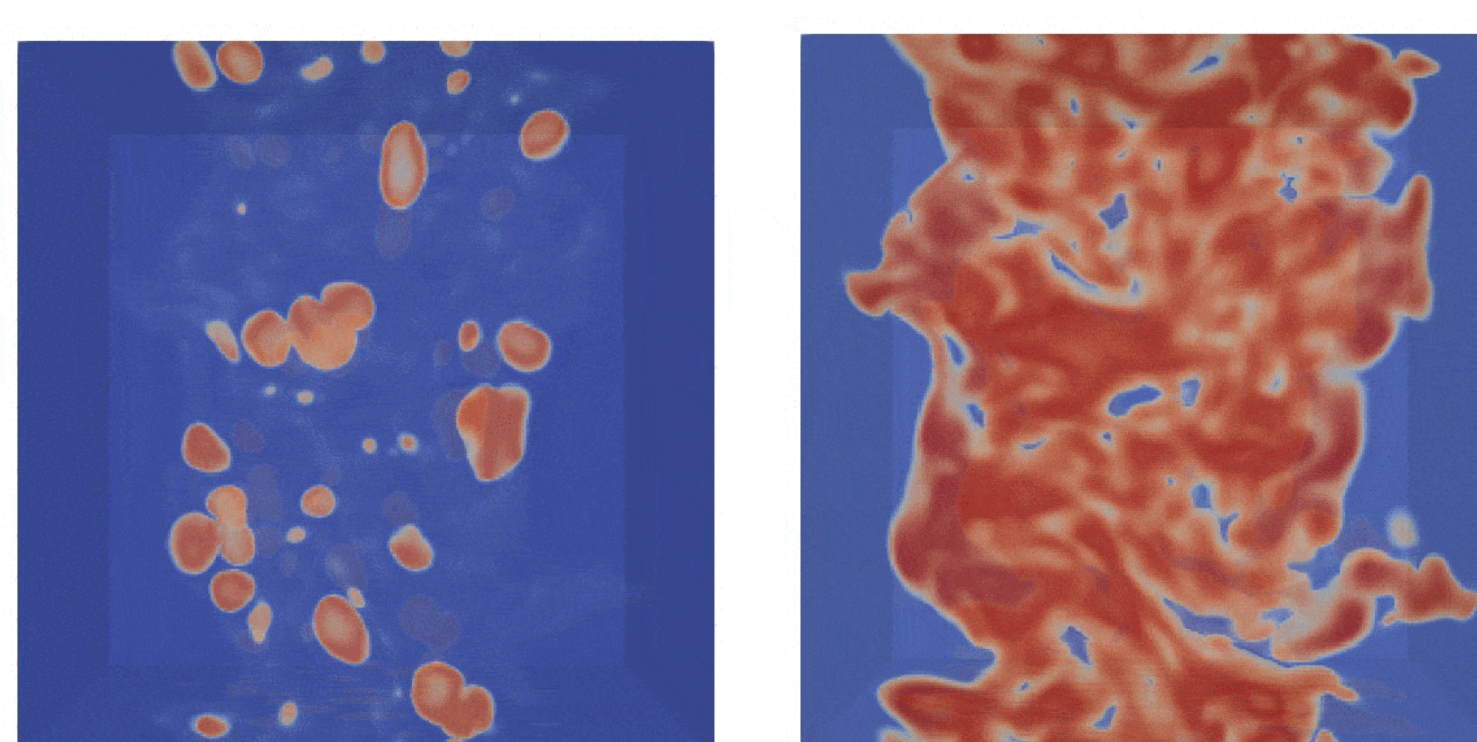
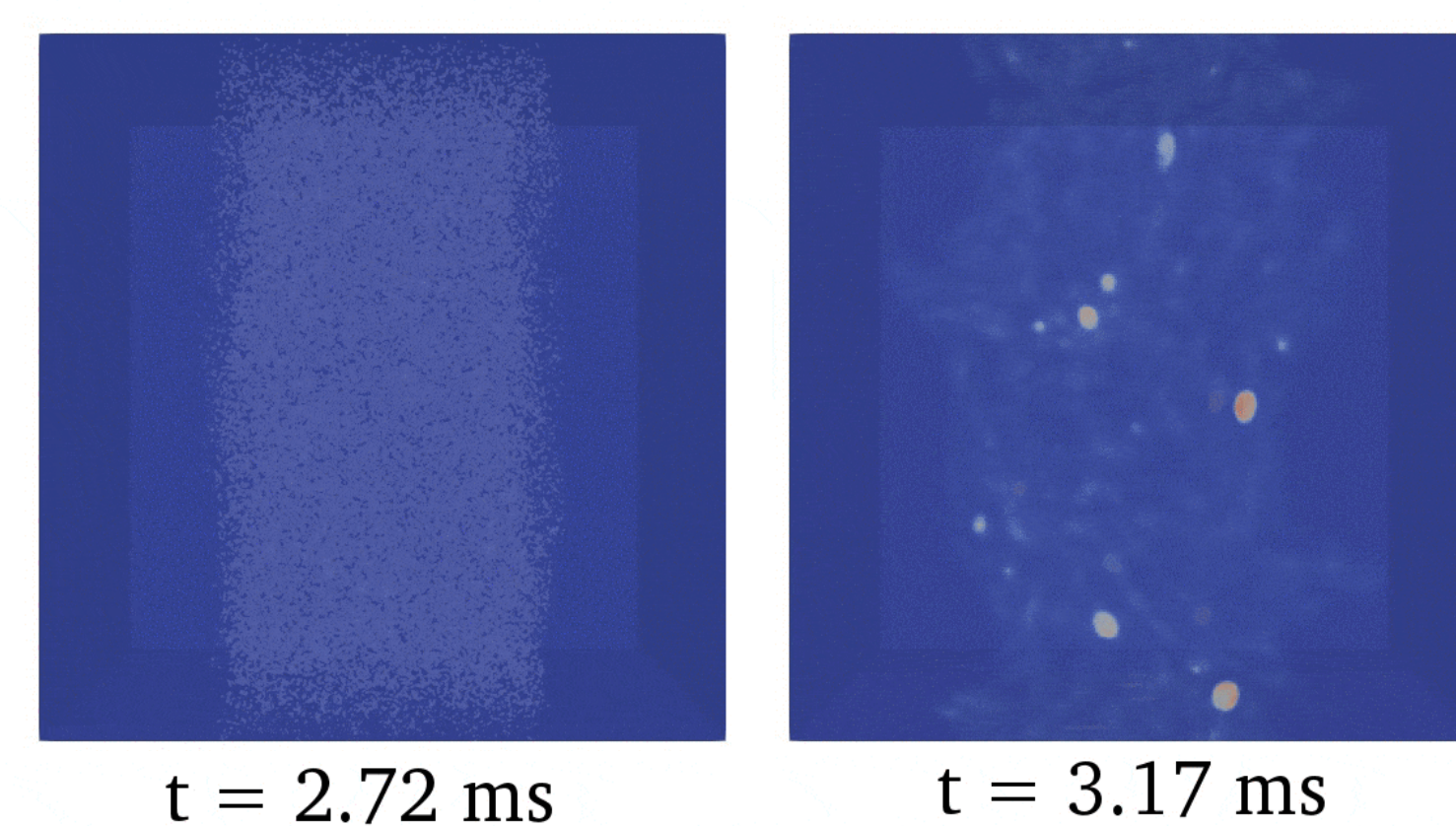
### Multicomponent evaporation and ignition

Transportation fuels consist of a large number of species that belong to different families of compounds. Predictions of physical and chemical properties of such multicomponent fuels require the accurate description of evaporation rates of all species initially contained in the liquid phase.

The group contribution model coupled to a multicomponent evaporation model is shown to accurately predict droplet evaporation rates for realistic jet fuels (below right).

The behavior of multicomponent spray ignition is investigated using DNS of realistic jet fuels. The behavior of the ignition kernel and subsequent propagation is shown (below left).

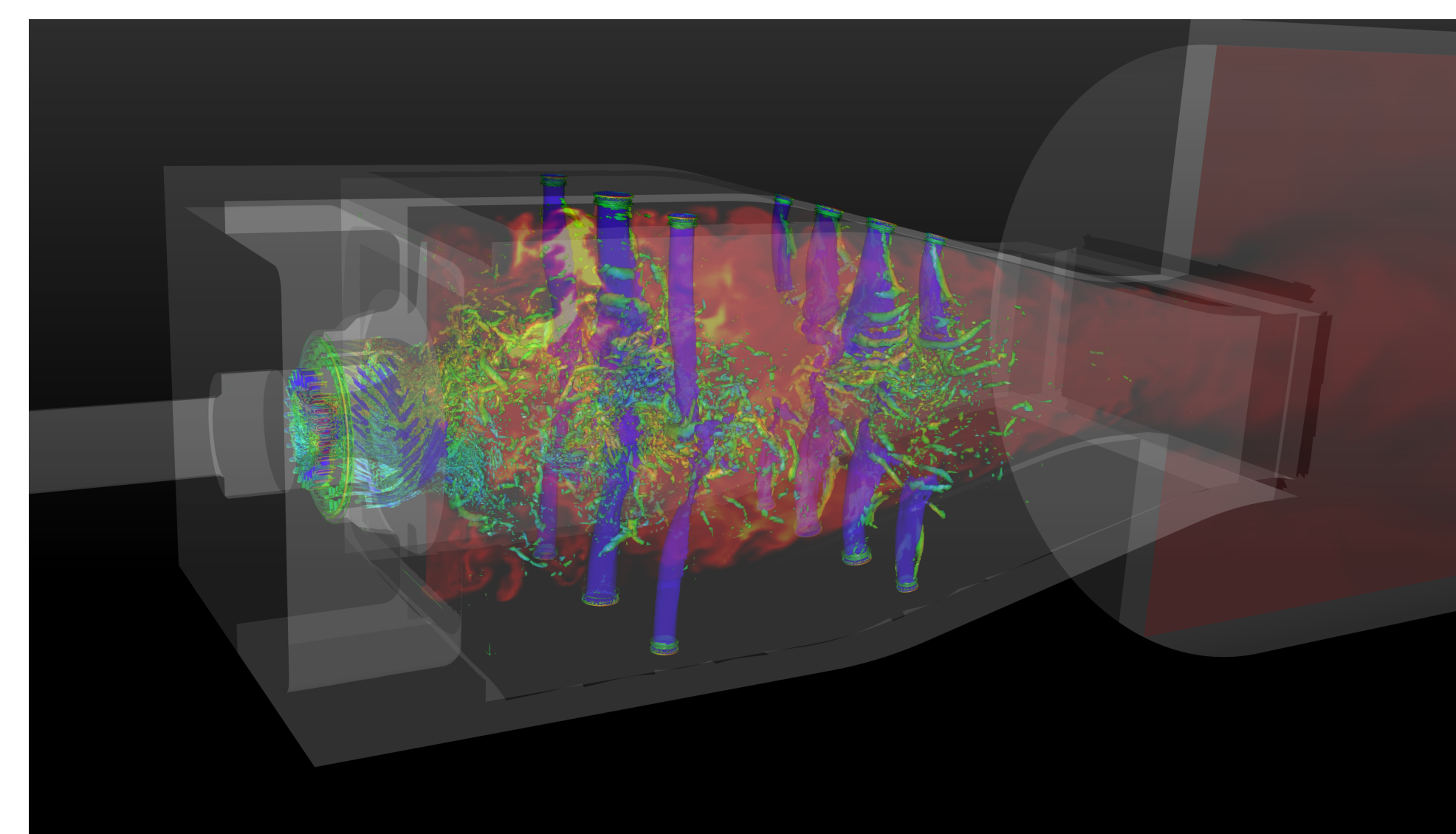
t = 1.00 ms      t = 2.38 ms



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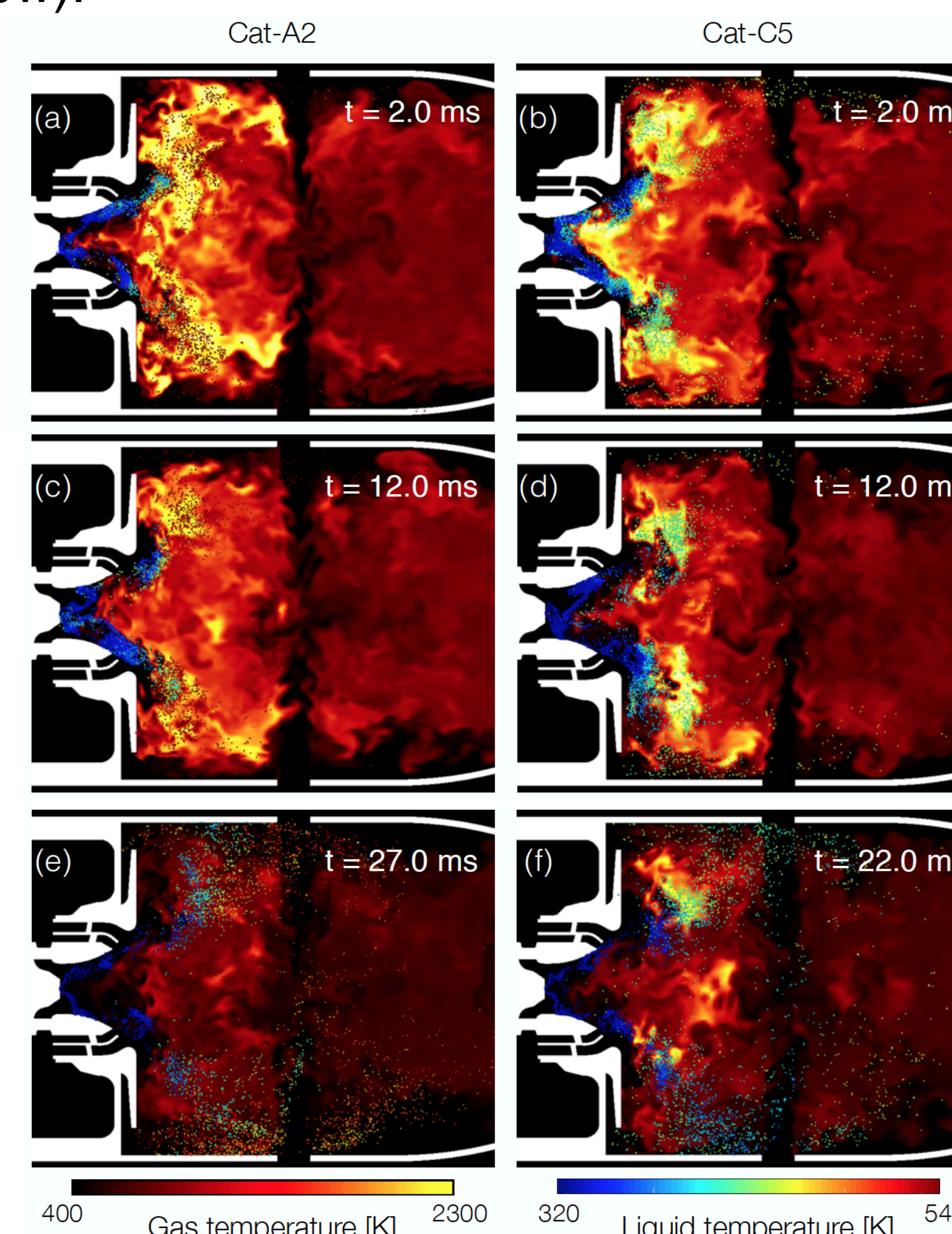
### LES of the LBO process

LBO behavior of candidate and reference fuels for the referee rig gas turbine is determined using LES. This engine contains the same major features of commercial engines and the same physical processes are observed.



The local temperature within the combustion chamber, the dilution jets and the vortex structure are shown for near LBO conditions (above).

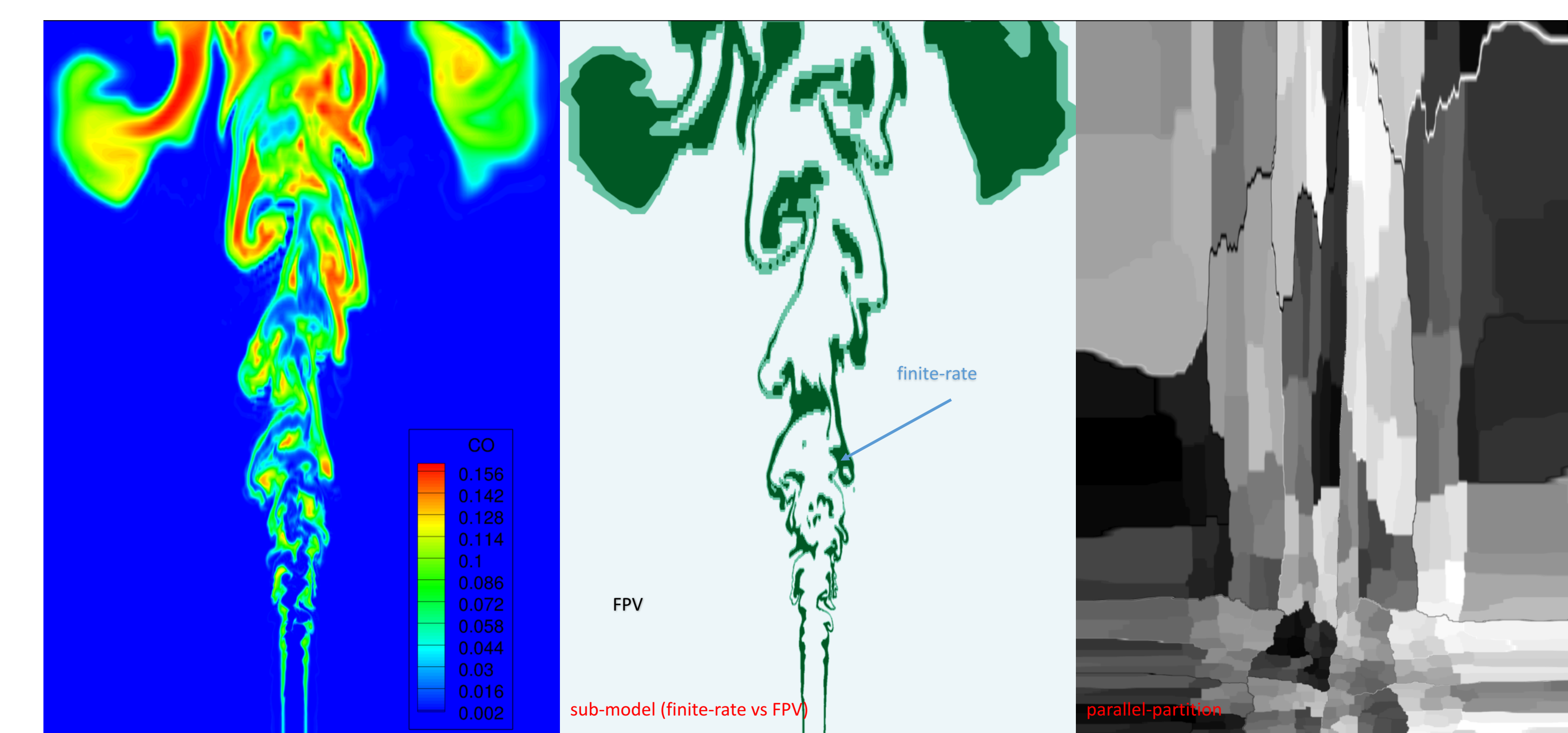
Transient LBO simulations are performed for two candidate fuels to investigate the fuel effects on LBO. LES shows that fuel effects can play a significant role in LBO behavior for gas turbines (below).



### Pareto-efficient combustion (PEC) model

The Pareto-efficient combustion (PEC) model combines highly accurate, but computationally expensive finite-rate combustion models with the computationally efficient but less accurate FPV combustion model.

By dynamically determining sub-model assignment a significant computational speed-up is achieved with minimal loss of accuracy. This is accomplished by determining the Parallel domain-decomposition based on sub-model costs resulting in balanced CPU load.



A DME Jet flame is simulated using a 30-species reduced mechanism along with a FPV model. Good agreement for the CO mass fraction is achieved with the current approach while reducing the computational load. The region where finite-rate chemistry is required is small in comparison to the computational domain. The load-balancing results in small flow-aligned domain partitions in areas where finite-rate chemistry is applied.

### Conclusion

- Multicomponent evaporation and ignition is required to better account for fuel effects.
- Transient LES of referee rig highlights the impact of candidate fuel on the physico-chemical processes responsible for LBO.
- The PEC model can reduce the computational time required to include finite-rate chemistry with minimal loss of accuracy.

### Next Steps

Application of PEC and multicomponent evaporation and ignition for referee rig.

Lead investigator: M. Ihme, Stanford University  
Research Team: H. Wu, P. Govindaraju, Q. Wang, J. Labahn, P. Ma.

Project manager: Cecilia Shaw, FAA  
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