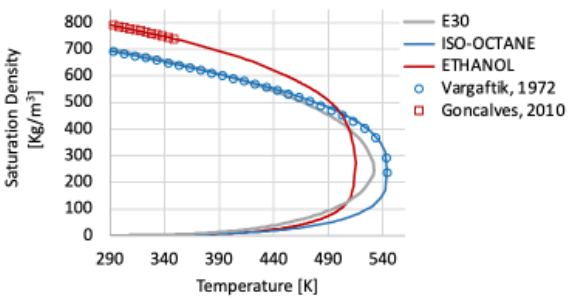
APPROACH

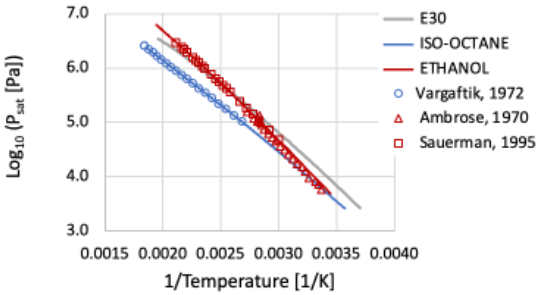
Connect thermo-physical properties to spray characteristics via high-fidelity simulations

SAND2021-12742PE

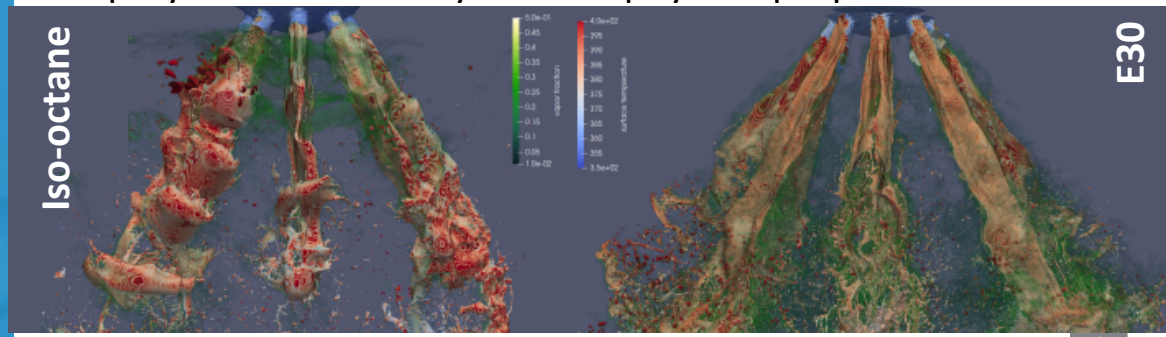
- Proceed with a methodology that minimizes the dependence on calibration from conventional fuels
- Create a small number of validated case studies using the real properties of the liquid/vapor/gas system (with SNL research code CLSVOF)
- From data, develop sub-models to cover gaps found in the engineering-level simulations

- Many fuel blends do not behave like ideal mixtures





- The primary atomization process is non-linear: focus on how sprays are affected by thermo-physical properties



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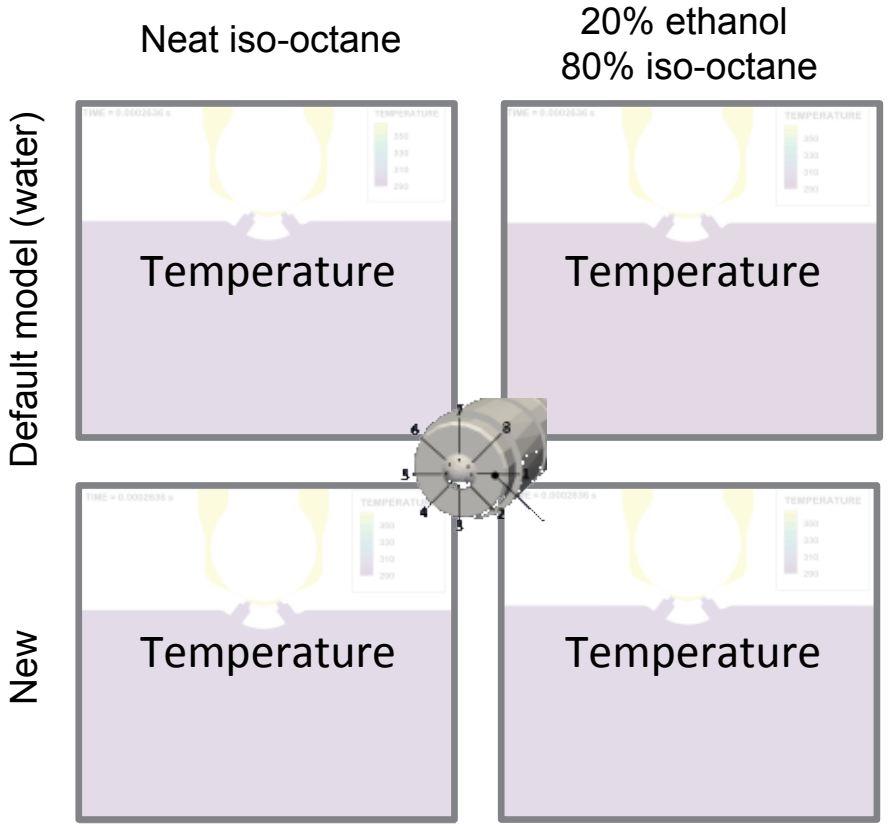
RESULTS

Improved sensitivity of CFD flash-boiling model to fuel blend composition

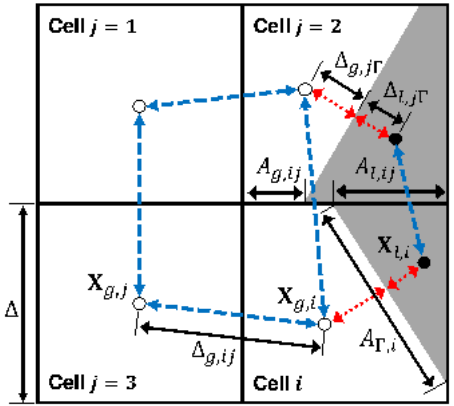
- The new Thermally-Limited Bubble Growth (TLBG) model helps distinguishing the effect of fuel composition on spray cone angle
- The new model is available in CONVERGE as user-defined function
- More progress possible by correcting the sound speed evaluation of the liquid-vapor mixture



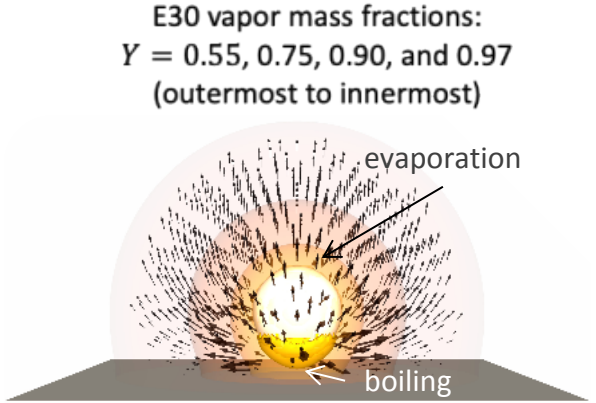
Arienti et al., "A thermally-limited bubble growth model for the relaxation time of superheated fuels," International Journal of Heat and Mass Transfer 159 (2020) 120089.

RESULTS Developed accurate surface evaporation model

- Predicts evaporation and boiling of real fuels without need of empirical correlations
- This implementation establishes the framework to examine the behavior of multi-component surrogates
- Added to CLSVOF without affecting existing solver's capabilities



- Diffusion and phase change are defined by a novel, operator-split methodology that is conservative and consistent in discrete form

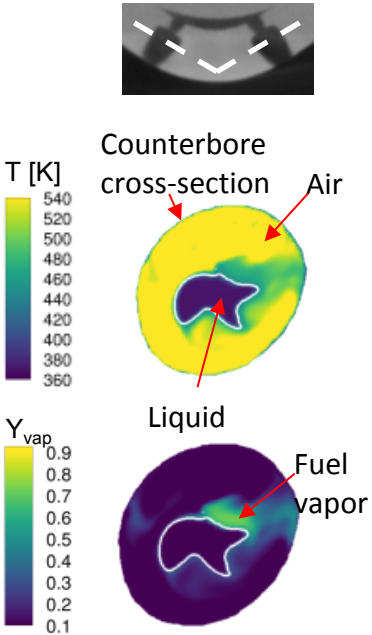


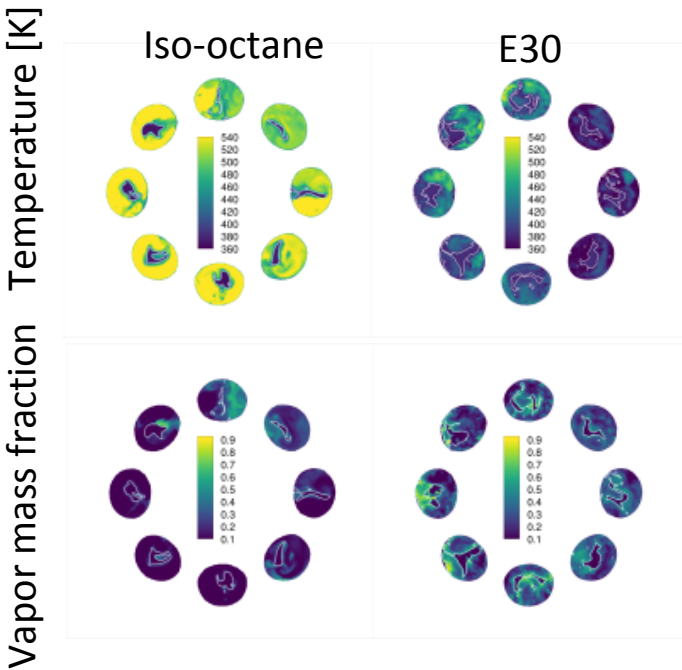
1. Wenzel and Arienti, "A new approach for the modeling and simulation of liquid/vapor phase change at engine-relevant conditions" Proceedings of the 31st ILASS-Americas, May 2021.
2. Wenzel and Arienti, "A conservative framework for the modeling and simulation of evaporation in compressible flow systems" In preparation for submission to *J. Comput. Phys.*

RESULTS

Case study: differences between neat iso-octane and E30 for GDI at end of injection

- Observed differences between two two fuels in spray angle and jet structure; much enhanced evaporation with E30
- Differences are particularly clear toward the end of injection as hot gas is entrained
- But with E30 the temperature increase at the liquid surface is mitigated by the cooling effect of evaporation





1. Arienti et al., ”Effects of detailed geometry and real fluid thermodynamics on Spray G atomization” Proceedings of the Combustion Institute 2021.
2. Arienti and Wenzel, “Detailed evaporation modelling for gasoline direct injection: iso-octane vs. E30,“ ACS Fall 2021.

Acknowledgements

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