The Development of a Deeper Understanding of Cantera for Use in the Simulation of Modern Combustion Problems

Shane Kosir (kosirs1@udayton.edu)

Advisor: Joshua Heyne, Ph.D.

Co-Advisor: Robert Stachler

Research Objective: To attain insight into ignition delay, a contributing parameter to lean blowoff (LBO), so that LBO can be used as a criterion for the selection of alternative jet fuels.

Introduction

Motivation:

- The development of alternative jet fuels (AJF) has been identified as an opportunity for economic, environmental, and national security purposes

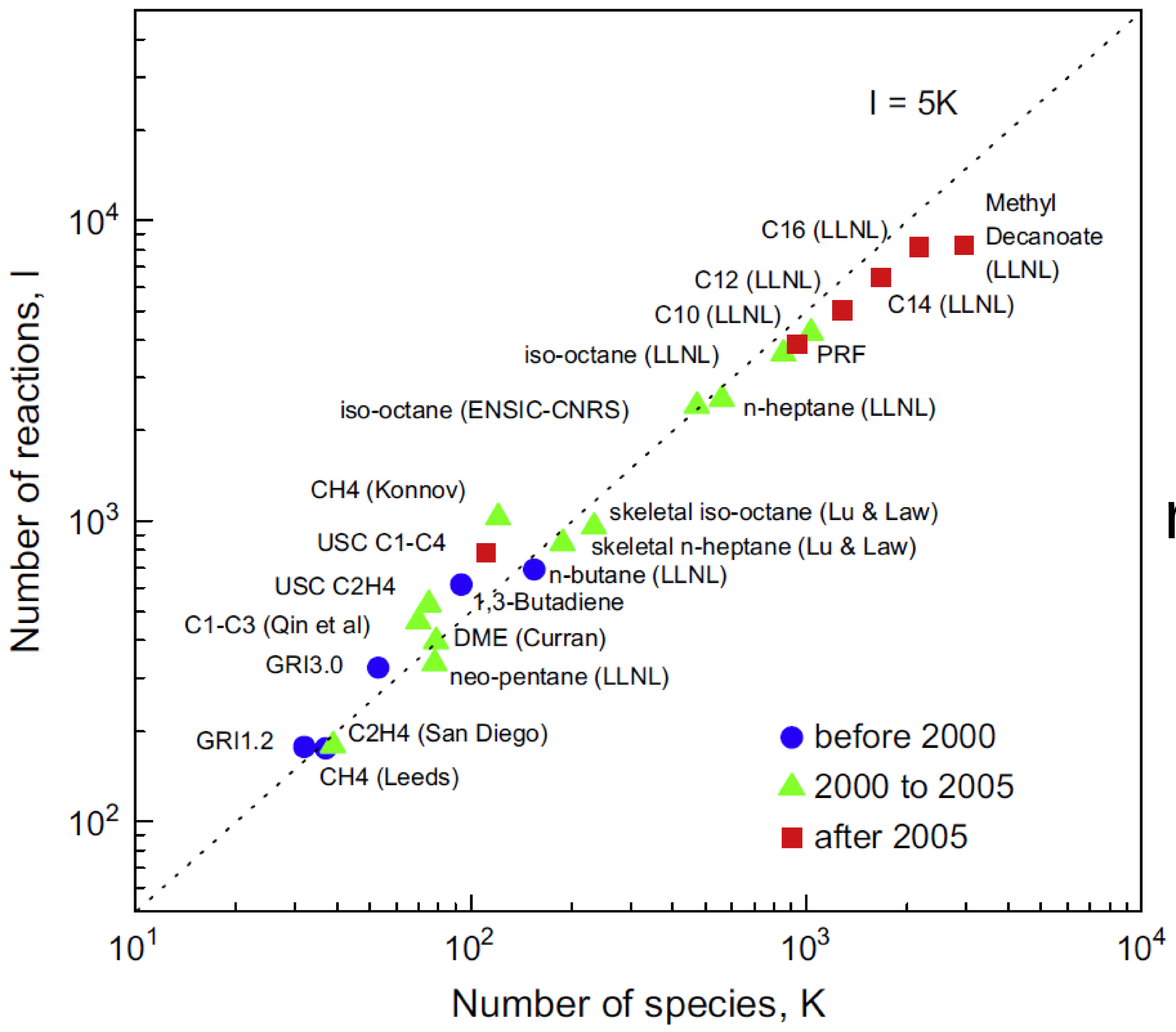
Current Limitation:

- The path to certification is arduous, with many fuel candidates unable to complete the certification process
- Simulation time to compare models to experiments is heavily increased by large fuel mechanism sizes to accommodate models of real fuels

Current Approach:

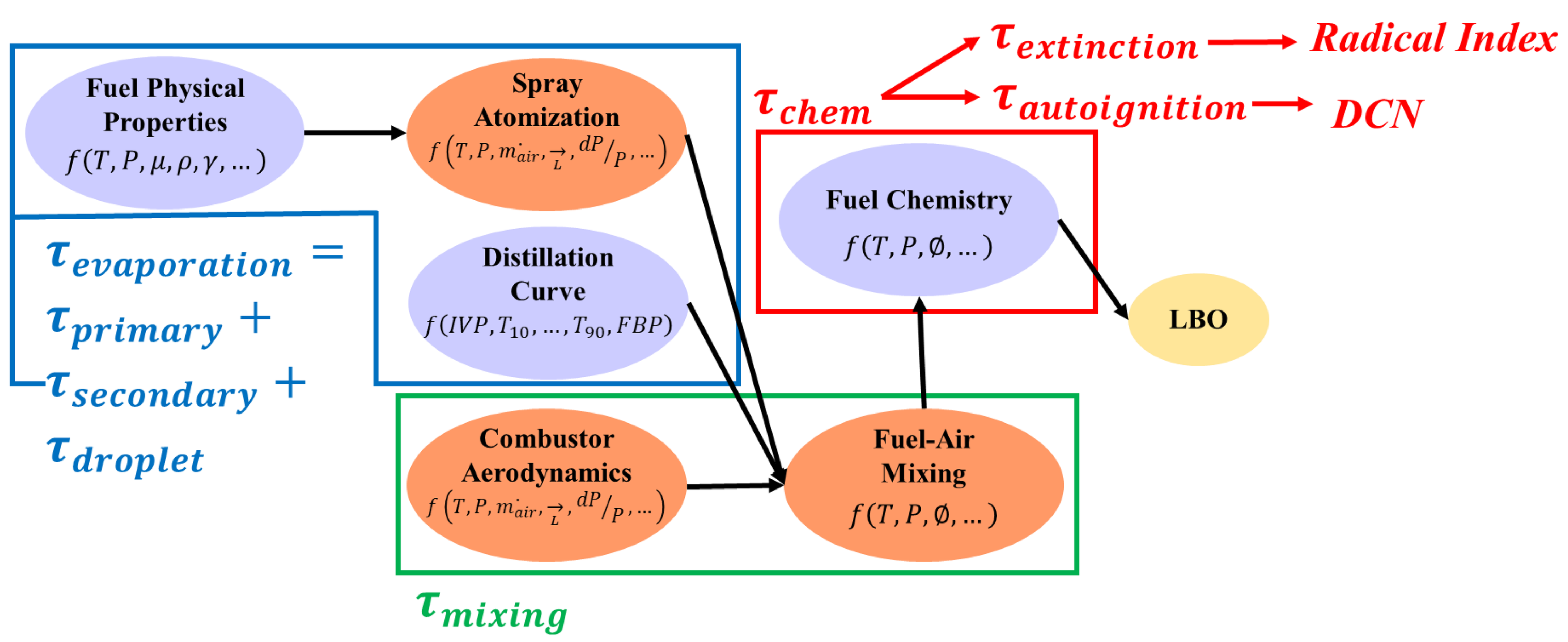
- The National Jet Fuels Combustion Program (NJFCP) is established to streamline the certification process by bounding the expected limits of conventional and alternative jet fuels for three key operability limits: cold start ignition, high altitude relight, and lean blowoff (LBO)
- LBO represents the lowest possible fuel-air mixture before a flame is extinguished

Hydrocarbon Mechanism Sizes (Lu and Law, 2009):



Detailed models of mechanisms are too large for simulation without reduction. More robust strategies for simulation can reduce computation costs and aid in the approval of AJF

Timescale Approach to LBO (Heyne et al., 2018):



$$\phi(LBO) \sim \left(\frac{1}{\tau_{chem}} + \frac{1}{\tau_{evap}} + \frac{1}{\tau_{mix}}\right)^{-1}$$

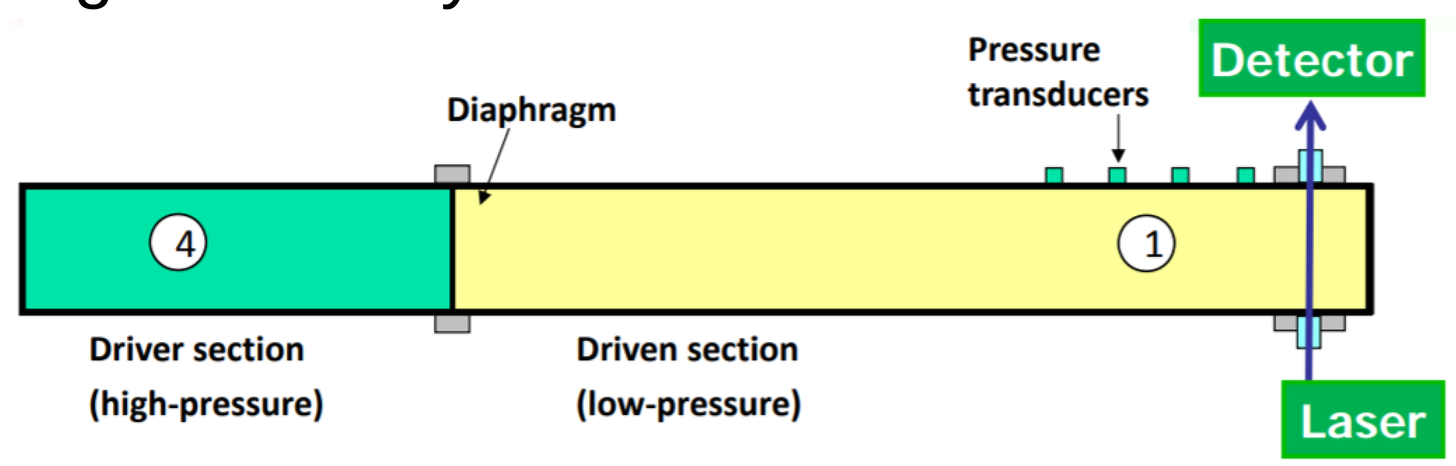
τ_{chem} and τ_{evap} relate fuel properties to LBO, while τ_{mix} relates combustor contribution to LBO

Connecting LBO Parameters:

$\tau_{\text{autoignition}} \rightarrow$ DCN $\rightarrow \tau_{\text{ignition delay}}$

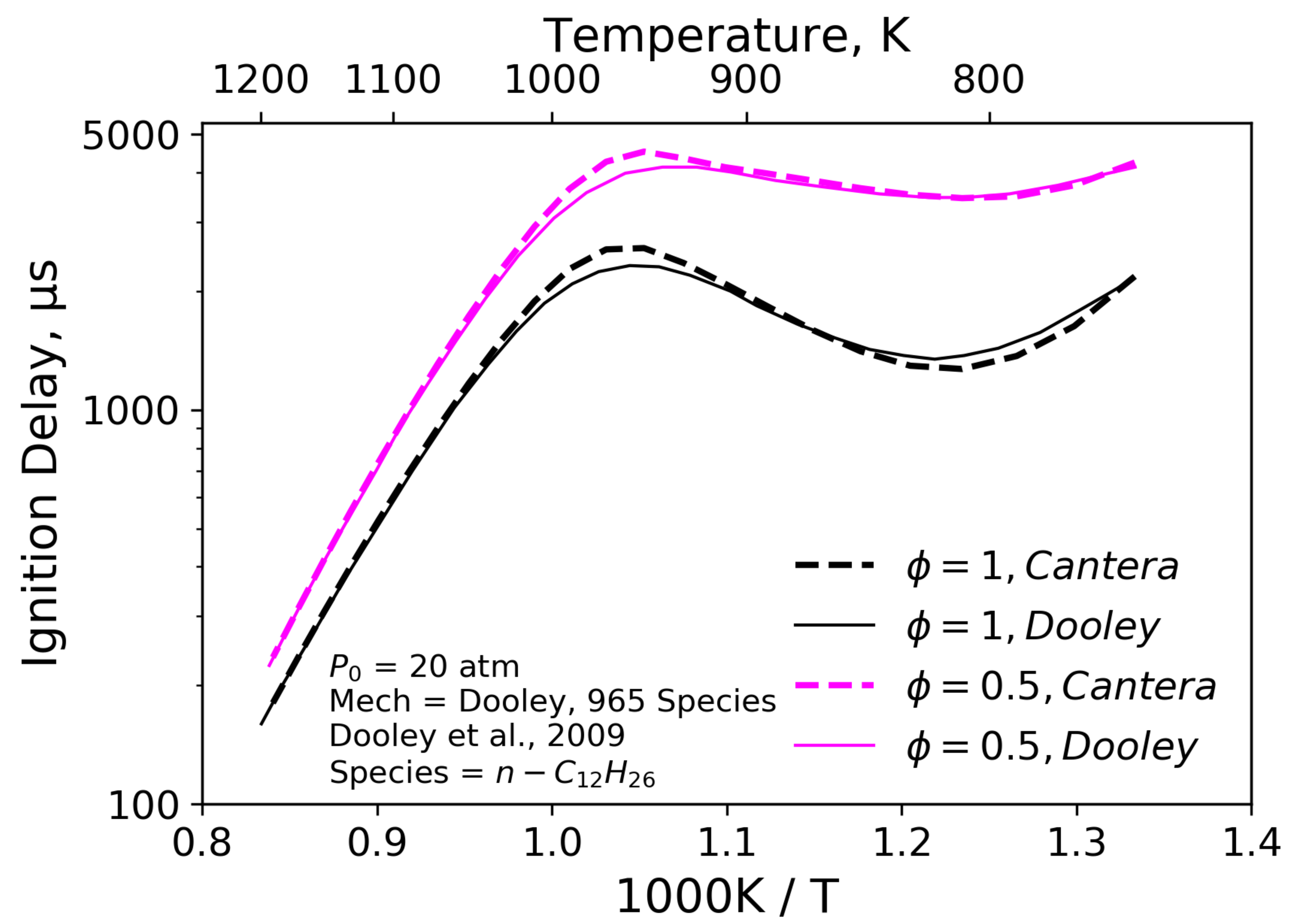
Methodology

- Cantera is software that is used to simulate problems involving thermodynamics, transport phenomena, and chemical kinetics
- Python code was developed using a constant-volume reactor in Cantera to calculate ignition delay
- One of the common experiments to measure ignition delay is via a **shock tube**



High-pressure gas expands, creating a shock wave and causing the combustion of the test gas

Results



Cantera simulations for the ignition delay of n-dodecane, an alkane hydrocarbon. n-dodecane has garnered attention as it is a typical n-alkane surrogate for kerosene-based fuels such as Jet-A and JP-8

Conclusions/Next Steps

- Current simulations yield similar results and validate simulation strategy used to calculate ignition delay
- Next steps include the creation of more robust code to simulate ignition delay for multiple mechanisms at various initial conditions (T, P, ϕ, fuel species)
- The goal is to reduce the amount of time required for ignition delay computation, which will aid in determining the connection between LBO and ignition delay

References

1. Dooley, Stephan, et al. “Reduced kinetic models for the combustion of jet propulsion fuels.” *51st AIAA Aerospace Sciences Meeting.* 2013.
2. Heyne, Joshua S., et al. "Year 3 of the National Jet Fuels Combustion Program: Practical and Scientific Impacts of Alternative Jet Fuel Research." *2018 AIAA Aerospace Sciences Meeting*. 2018.
3. Lu, Tianfeng, and Chung K. Law. "Toward accommodating realistic fuel chemistry in large-scale computations." *Progress in Energy and Combustion Science* 35.2. 2009.