Popular summary in English

The aviation industry releases 2.5% of global CO_2 emissions and is a major contributor to climate change. Reducing these emissions is challenging due to the design requirements placed on aircraft engines: electric motors and fuel cells are too heavy for larger aircraft, while hydrogen-burning jet engines are difficult to implement safely and reliably. However, there is hope in the form of Sustainable Aviation Fuel (SAF), i.e., renewable biofuels that can be used in conventional jet engines.

SAF can be produced in many ways. Some methods synthesize it from alcohol and sugar. Others use waste products like sewage or used cooking oil, giving the fuel a very low environmental footprint. Others still use biological byproducts from industrial processes; important examples of this in Sweden include forest residues or byproducts from paper production. The fuels produced by this wide range of methods and materials can vary greatly in composition and lack some important features of established fossil fuels. A general trend is a lack of aromatics, carbon rings that are naturally plentiful in petroleum and fossil fuels, which are necessary for proper lubrication and seal swelling in jet engines. For these reasons, SAF is only certified for use in aircraft when blended with fossil fuels up to a maximum ratio of 50/50.

When more than 50% SAF is put into the tank, the differences between it and conventional fuel can start to become noticeable. However, the effects of these differences are not well known because our scientific and practical experience burning SAF is minuscule compared to fossil fuels. There is an urgent need for research on how SAFs burn so that blending limits can be increased and new production methods can be certified. To gain as much knowledge as possible, it should not only be done with traditional experiments but also with detailed computer simulations. Simulations can provide data that is unobtainable using experimental measurements and allow for predictive and exploratory studies that generate new theories. Large Eddy Simulations (LES) are one such simulation technique, well-suited for studying the complex and turbulent combustion inside a jet engine, as it constructs a full 3D model of the constantly shifting flame. Although powerful, LES requires an astronomical amount of calculations, which makes access to a supercomputer a necessity.

This work uses LES to study the combustion of several jet fuels, including SAF. The set of fuels represents a wide range of characteristic properties like density and aromatics content, and each fuel is used in its pure form. In this way, the effects of the different properties become as impactful and measurable as possible, making it easier to connect them to the different combustion behaviors of each fuel. Two different cases are studied. Case A is a simple lab-scale burner, somewhat similar to a camping stove, where the fuel is fully vaporized and mixed with air before igniting. Case B is a generic model of a real jet engine combustor and includes many features of real engines, such as air pressures up to ten at-

mospheres, direct injection of liquid fuel into the combustion chamber, and swirlers that induce rotation in the flow to stabilize the flame. Both cases have previously been used in experiments elsewhere, and their results are publicly available. The LES model reproduces the available results very well, indicating that the modeling methodology is well-suited to the problem.

In case A, the simulations reveal several distinct fuel trends. The temperature at which each fuel burns decides the overall size of its flame, which is very useful information since the flame temperature can be easily calculated without either experiments or simulations. The ignition quality of each fuel, which is measured using the Cetane Number (CN), appears to influence how steady the flame is, with low-CN fuels having steadier flames than high-CN fuels. A hypothetical explanation for this unexpected result is formulated using chemical time scales, and further research will show how well it holds up.

In case B, the simulations show that the different fuels behave quite similarly when the engine is run in idle mode, but distinct differences emerge in cruise mode. The most important factor is the vaporizability, which is a measure of how easily the liquid fuel is broken up into small droplets and then turned into vapor. The more vaporizable fuels have more compact flames and burn closer to the fuel injector. This increases the fuel-to-air ratio where the chemical reactions happen, which in turn increases the flame temperature. Because the flame temperature is so high, the nitrogen in the air reacts with the oxygen to form nitrogen oxides, NO_x , which are harmful to both people and the environment. The more vaporizable fuels also give rise to strong pressure waves that make their flames less stable and put the engine under stress.

The combined results of this work demonstrate how radically different fundamental fuel properties lead to different combustion behaviors. As more experiments and simulation studies are carried out, the range of possible SAF properties and their effects will be mapped out and understood. This understanding should pave the way for higher blending limits with some SAFs and allow new production methods to enter the market.