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Modeling the kinetics of the Shockless Explosion Combustion

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ABSTRACT

The Shockless Explosion Combustion (SEC) is a novel approach to approximating constant volume combustion in gas turbines. It promises an efficiency gain comparable to that of pulse detonation combustion without the drawbacks associated with detonations. It utilizes quasi-homogeneous combustion of a volume of fuel & air mixture to avoid strong shock waves, similar to the Homogeneous Charge Compression Ignition (HCCI) process in internal combustion engines. Recharging is handled in analogy to a pulse jet combustor through resonant pressure waves in the combustion chamber. To achieve nearly homogeneous auto-ignition, a stratified layer of fuel/air is set up such that almost constant time to ignition remains across the charge once the recharging process is completed. Here we introduce simplified chemical kinetics models that enable efficient computational modeling of the entire process. Based on numerical simulations we assess essential influences of chemical kinetics on the subtle gasdynamics involved in the SEC process and discuss results on its feasibility.

1. Introduction

The Shockless Explosion Combustion (SEC) is a promising operation mode for gas turbines that was introduced in [1]: By carefully tailoring a fuel/air stratification inside a combustion chamber at a temperature close to the auto-ignition temperature, a mixture can be set up to homogeneously self-ignite. This leads to approximate constant volume combustion (CVC). Compared to the classical Brayton cycle, in which a steady flame leads to approximate constant pressure combustion, CVC offers a significant efficiency increase [2]. This is a well-known fact, and hence other pressure-gain combustion cycles are under investigation by the community. Most notably, the pulsed detonation combustion (PDC) utilizes detonations to achieve approximate CVC. It suffers from several theoretical drawbacks that the SEC avoids: Detonations are associated with strong shock waves that are undesirable in a machine. Also, a certain amount of the fuel in a PDC cycle must be burnt deflagratively, because after ignition, the flame must first be accelerated sufficiently to obtain a detonation, in a deflagration to detonation transition (DDT) [3]. The SEC utilizes the combustion tube as a resonator for the pressure waves that the combustion generates, similar to the acoustic Rijke tube experiment. If properly tuned, the waves are sufficiently strong to generate the current required for recharging the tube for the next cycle, which allows a machine utilizing the SEC to work with few mechanical parts. A conceptual precursor to this charging concept is the pulse jet engine, which is based on the same principle. It does not combine it with the use of auto-ignition for ignition, but rather combusts its charge in a turbulent flame [4].

The SEC is quite similar to the HCCI process in internal combustion engines, where one attempts to homogeneously combust a charge using compression ignition [5]. Both processes require fine-grained control over the charge to achieve homogeneous combustion, though with different optima: In the HCCI, one aims for a homogeneous charge which is then compressed and eventually self-ignites. In the SEC, the fuel/air mixture is created already close to auto-ignition, and a stratification must be deliberately created to account for the different residence times of the fuel, and thus achieve homogeneous auto-ignition. Both processes eventually involve an auto-ignition that may either be regarded as approximately homogeneous, or as a deflagrative or detonative combustion process, depending on gradients in the stratification of auto-ignition delay time upon ignition. For the HCCI, this has been investigated thoroughly (*e.g.*, [6]), and also for the abstract case of general auto-ignitions of stratified mixtures, numerical and theoretical results are known [7]. The general mechanism, which plays a role in DDT as well, is called Shock Wave Amplification by Coherent Energy Release (SWACER), and was first described in [8]. The theory basically states that if a gradient in auto-ignition delay time is present, then a chemical auto-ignition wave will travel through the mixture, with the point where the mixture currently ignites at its front. If this wave has the correct speed to couple with the pressure rise due to combustion, a detonation forms. If it is too slow, combustion is deflagrative. If it is sufficiently fast, a

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weak detonation, or in the limit case a thermal explosion, occurs. The latter is what we aim for in the SEC.

The charging process of a SEC hence is of particular interest. A parameter of the fuel injection, such as the fuel/air ratio, must be continuously adjusted such that at some given time the remaining ignition delay time of the entire mixture is "sufficiently" homogeneous in space. In [7,9], the authors show that distinct limits for the strength of the auto-ignition delay time gradient exist that separate the desired constant volume explosions from detonations that we wish to avoid: For our purposes, we demand that the gradient is such that the speed of the auto-ignitive reaction front exceeds that of a Chapman–Jouguet detonation.

Ignition delay times depend on the chemical composition, stoichiometry and thermodynamic properties of a mixture. Close to the auto-ignition temperature, temperature dependence is typically the strongest, and simultaneously hard to control in experiments to the precision required due to that dependence. For the SEC, it has therefore been proposed to use a fuel that is tailored to significantly reduce this dependence by utilizing the negative temperature coefficient (NTC) behavior of certain hydrocarbon fuels, *i.e.*, that in a region of initial temperatures the ignition delay time increases with increasing initial temperature [10]. The aim is to have a fuel whose auto-ignition delay time varies only on the scale of milliseconds over a range of about 100 K. Since the chemical composition is fixed by that choice, the delay times must then be controlled through the stoichiometry, which can be easily adjusted in principle by opening the fuel value to a certain amount while charging. In particular, it has been suggested to include Dimethyl Ether (DME, CH_3OCH_3) in the final fuel.

In terms of chemical kinetics, a fuel blend with largely temperature independent auto-ignition delay times achieves this independence by means of a balance of various concurring reactions with different reaction paths. Traditional models for such fuels, based on a series of reactions with rates described by Arrhenius equations and more elaborate expressions for third-body reactions, hence necessarily do not admit reduction to very few reactions without losing this property: A reduction of the mechanism from [10] did not allow less than 83 species with 1% error on the experimental auto-ignition delay times, or 33 species with 10% admissible error, respectively. It is desirable to have a small model though: For one, it enables long-time, resolved fluid dynamical simulations and parameter studies that are too expensive with complex mechanisms. For the other, a small model can be used for qualitative investigations yielding general results on admissible fuels, because it only has few parameters and is easy to conceptually understand. This latter purpose is of particular interest, because the search for suitable fuels for a SEC is ongoing. Constraints found using a general, qualitative model apply to all possible fuels, and hence allow to refine the requirements and, thereby, narrow the search.

This paper therefore introduces a model for fuels with temperature-independent ignition delays times, and shows by means of numerical studies that a SEC is readily achievable once a suitable fuel has been found. We then present parameter studies that identify the error tolerances in an ideal SEC and on SEC-suitable fuels. We conclude the paper by showing that the sensitivity requirements on the fuel are entirely of technical nature, by means of a simulation of a SEC using H_2 as a fuel: The required temperatures and accuracies are too high for current technical purposes, but if achieved, according to the available models, would yield a SEC as expected.

2. Model

In this section we construct a computational model for a SEC in the combustion chamber of a gas turbine that lies between a compressor plenum and a turbine plenum, both ideal in the sense that they have a fixed pressure. We assume that the mixing is sufficiently efficient to model the SEC tube as radially homogeneous, reducing the problem to one effective space dimension. The model will be implemented in a finite volume framework using ghost cells for the boundary conditions. It therefore suffices to prescribe the state at the boundaries: The upstream end is sealed using a fluidic diode [11] to prevent pressure waves from running upstream into the compressor plenum. We assume ideal diodicity and model it as a boundary that reflects perfectly as long as the inside pressure exceeds the compressor plenum pressure and otherwise takes the thermodynamic state of an isentropic and isenthalpic expansion of the plenum state to the inside pressure, with the excess enthalpy transformed into kinetic energy. Mixing of fuel and air is not part of the model, instead we assume that mixing occurs instantaneously at the tube inlet. At the downstream end, the turbine plenum is modeled as an instantaneous increase in diameter to infinity: The (one-dimensional) plenum exit hence has fixed pressure. Since upon transition from the pipe to the plenum, gas can expand in all directions, we assume that velocity does not change significantly in axial direction at the outlet. The downstream state therefore is obtained by isentropic expansion to the plenum pressure, neglecting any excessive energy.

The fuel stratification in a SEC has a short residence time due to the low auto-ignition delay times in the order of milliseconds. When it is created, the flow on average has a Mach number of about $\mathrm{M} = 0.4$, resulting in a characteristic Reynolds number of about $\mathrm{Re} = 8 \cdot 10^6$ for the charging process. This allows to neglect diffusion in the simulation of the SEC.

Fluid dynamics is therefore represented by the one-dimensional Euler equations with additional continuity equations for the partial masses of the different species, and chemical source terms, *i.e.*,

$$\begin{pmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y_i \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(\rho E + p) \\ u \rho Y_i \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ \rho \dot{E}_{\mathrm{chem}} \\ \rho \dot{Y}_{\mathrm{chem}} \end{pmatrix}, \tag{1}$$

with density ρ, velocity u, pressure p, energy $E = \frac{1}{2}u^2 + e(\rho, p)$ with internal energy e and mass fractions $Y_1 \dots Y_n$ that are normalized to sum to unity. The equation of state, in form of an expression for e, closes the system. It is given either by the ideal gas law for gas mixtures, or, in case of our idealized fuel model, by the perfect gas law $e = p/(\rho \cdot (\gamma - 1))$ with isentropic expansion factor $\gamma = 1.28$. The value corresponds to that of an stoichiometric DME/air mixture. For the calculations using the reduced bottom-up models introduced below, this system is nondimensionalized by choice of the outer pressure p_0, length of the tube ℓ_0 and average ignition delay time t_0 as reference quantities, and by division of the first equation by reference density $\rho_0 = p_0 \ell_0^{-2} t_0^2$, second equation by $\rho_0 u_0$, with the reference velocity given by $u_0 = \ell_0 t_0^{-1}$, and third equation by p_0. The chemical source terms $\dot{Y}_{\mathrm{chem}}$ and $\dot{E}_{\mathrm{chem}}$ are given by a set of reactions transforming reactants to products, with associated reaction rates r, releasing an amount of energy of ΔQ. In the special case of the simple models that will be introduced below, a reaction's reactants and products may be described by two vectors R and P, containing a 1 for each species that occurs on the corresponding side of the reaction equation, and a 0 otherwise. The expressions for both terms are then:

$$\dot{Y}_{\mathrm{chem}} = \sum_{i \in \mathrm{reactions}} (P_i - R_i)\, r_i, \tag{2}$$

$$\dot{E}_{\mathrm{chem}} = \sum_{i \in \mathrm{reactions}} (\Delta Q)_i\, r_i. \tag{3}$$

Fluid dynamics and chemical kinetics are solved separately using Strang splitting. The fluid dynamical part of the system is solved using a finite volume method with second order MUSCL (short for

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