



Tabulated chemistry approach for diluted combustion regimes with internal recirculation and heat losses



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ABSTRACT

An efficient solution to reducing NO_x formation is to maintain a relatively low flame temperature. This can be achieved by mixing reactants, prior to combustion, with chemically inert diluents such as cooled combustion products. In such diluted combustion systems, the flame temperature decreases because of thermal ballast, limiting NO_x production. This work focuses on modeling the specifics of this combustion regime in confined combustors. To characterize the dilution of reactants by burnt gases, the importance of complex chemistry effects is emphasized and taken into account using a detailed chemistry tabulation approach. This approach extends the flamelet/progress variable formulation by including information about the intensity of internal dilution rates and heat losses. A turbulent combustion model is then developed in a large eddy simulation (LES) framework. The combustion model is validated by considering two combustor configurations, namely an adiabatic burner and a combustor having isothermal walls – both operating under highly diluted combustion conditions. Simulation results are in good agreement with experimental data, confirming the importance of detailed chemistry information and the validity of the tabulation approach to LES application to diluted combustion.

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1. Introduction

The energetic efficiency of combustion systems can be enhanced by transferring heat from exhaust products to the fresh gases by means of regenerative heating. Unfortunately, the resulting increase in the reactant temperature has an adverse effect on the formation of nitrogen oxides (NO_x). An efficient solution to reducing NO_x formation is to maintain a relatively low flame temperature. This can be achieved by mixing reactants with chemically inert diluents such as combustion products. In “diluted combustion” systems, the flame temperature decreases because of thermal ballast, limiting NO_x production. These systems promote different combustion regimes such as MILD (moderate or intense low-oxygen dilution) combustion [1,2], flameless oxidation [3] and high-temperature air combustion (HiTAC) [4,5].

In diluted combustion technologies, reactants are diluted with large amounts of burnt reaction products prior to combustion, which enables flame stabilization under lean conditions, thereby avoiding high-temperature regions that promote enhanced

thermal NO_x formation. Experimental and numerical studies have been conducted in confined systems such as HiTAC combustion chambers [6,7], the IFRF (International Flame Research Foundation) semi-industrial-scale configurations [8–10], and reverse flow configurations [11,12]. These diluted combustion technologies exhibit strong recirculation zones that enhance the mixing between fresh and burnt streams. Local stoichiometric conditions are avoided, so that NO_x production is dramatically decreased. It is noteworthy that diluted combustion can be achieved without internal recirculation of burnt gases: for example, Dally et al. [13] reproduced oxygen-diluted and MILD combustion regimes in a Jet in Hot Coflow (JHC) experiment.

A schematic of the model problem of diluted combustion with internal product gas recirculation in a confined burner geometry is shown in Fig. 1. The schematic illustrates the modification in the composition of reactants, which strongly varies with recirculation and dilution by burnt gases.

A major issue in the modeling of diluted combustion is the pronounced sensitivity of the flame structure to the reaction chemistry [14,15]. To illustrate the importance of the detailed chemistry when a gas mixture is subjected to dilution by hot reaction products, a series of adiabatic laminar flames are computed. These simulations consider chemical representations of increasing

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Nomenclature

Latin

C	normalized progress variable
D	molecular diffusivity
H	specific mixture enthalpy
S_Z	mixture fraction unmixedness factor
T	temperature
Y_c	progress variable
Y_D	dilution variable
Y_e	elemental mass fraction
Y_k	species mass fraction of species k
Z	mixture fraction
Z	mixture fraction normalized with respect to undiluted compositions

Greek

α	dilution parameter
β	heat loss parameter
Λ	progress parameter
ρ	density

ϕ	equivalence ratio
ϕ_G	global equivalence ratio
χ	scalar dissipation
ψ	vector of chemical quantities
$\dot{\omega}$	vector of chemical reaction rates, expressed in s^{-1}
$\dot{\omega}_k$	chemical reaction rate of species k , expressed in s^{-1}

Superscripts

Dil	diluent stream
F	fuel stream
Ox	oxidizer stream
0	undiluted conditions

Subscripts

G	global equivalence ratio conditioning
$ \alpha=0$	undiluted-conditioned quantity
$ \beta=0$	quantity evaluated without heat losses ($\beta = 0$)
$ \beta=1$	quantity evaluated for maximal heat losses ($\beta = 1$)

complexity, namely the infinitely fast chemistry approximation, a one-step irreversible chemistry, and a detailed reaction sequence. The problem configuration consists of a steady-state counterflow methane/air diffusion flame, and different values of strain rates (including the stable and the unstable branch) are considered. Both reactant streams are diluted with burnt products, having a composition that is identical to that of the MILD combustor configuration studied by Verissimo et al. [16] (see Section 5.1). Chemical trajectories in CO_2 – CH_4 composition space are presented in Fig. 2 for different dilution levels. Results obtained with the detailed GRI 3.0 mechanism [17] are shown by solid lines, the dashed line corresponds to the one-step irreversible chemistry, and the limiting case of infinitely fast chemistry is shown by the symbol. From this figure it can be seen that the detailed chemistry solution exhibits several possible trajectories, which depend on the level of dilution. In contrast, the single-step chemistry trajectory is not sensitive to the dilution level, so the CH_4 mass fraction exhibits a linear dependence on Y_{CO_2} . Since the infinitely fast chemistry model assumes that the mixture is always at equilibrium state, the chemical trajectory reduces to a single point for a given value of equivalence ratio. Results from the detailed chemistry solution show that the chemistry is affected by dilution, impacting fundamental flame properties, including flame structure, species composition, and pollutant emission.

An attractive strategy for including detailed chemistry effects using moderate CPU resources are tabulated chemistry techniques

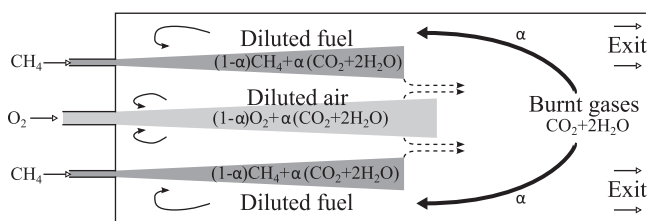


Fig. 1. Model problem of a diluted combustion configuration with internal recirculation of burnt gases. Considering the idealized problem of methane/oxygen combustion, the initially separated reactants mix and react to produce CO_2 and H_2O . Reaction products are then recirculated where they modify the composition in the oxidizer and fuel streams. The product gas dilution level is denoted by α .

[18–22]. Among these, the flamelet model for nonpremixed combustion assumes that a turbulent flame can be decomposed into a collection of one-dimensional flame elements [18]. Each flamelet is then represented by a reaction–diffusion element that is constructed between oxidizer and fuel streams. In the original formulation, proposed by Peters [18], the fuel and oxidizer composition are assumed to be constant for each flame element. By construction, this two-stream formulation is not able to account for effects of reactant dilution by burnt gases on the chemical flame structure. To overcome this issue, a three-stream flamelet-progress variable (FPV) approach has recently been developed [23]. This model was applied to large eddy simulations of a Jet-in-Hot-Coflow (JHC) burner [23,24], in which the burner was operated in the recirculation-free adiabatic MILD operating regime. The dilution

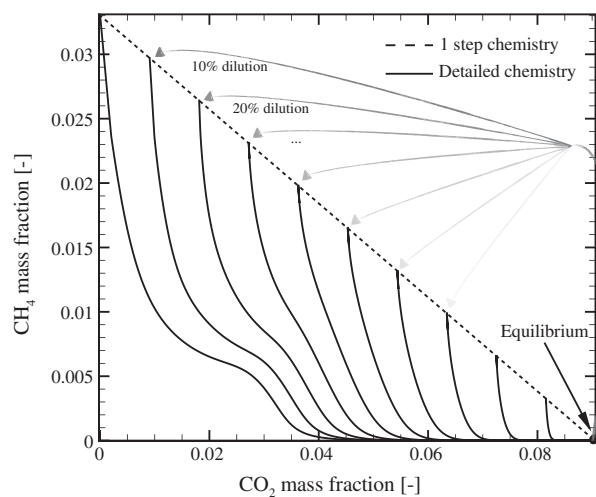


Fig. 2. Chemical trajectories in CO_2 – CH_4 state space for different dilution levels, illustrating the sensitivity of the fuel conversion to the reaction chemistry and the dilution. Here, the diluent is composed of the equilibrium product-gas composition for an equivalence ratio of $\phi = 0.58$. Trajectories are extracted from steady laminar counterflow diffusion flame computations, from the pure mixing line to the fully burnt states.

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