# Controlled Combustion—An Approach for Reducing Irreversibilities in Energy Conversion

**Investigators:** Craig T. Bowman, Professor, Department of Mechanical Engineering; Neelabh Arora, Kevin Walters, Graduate Research Assistants

**Sponsor:** Global Climate and Energy Project (Completed 12/31/05)

**Final Report Online**: http://gcep.stanford.edu/research/technical_report.html

**Introduction:** Energy specific $CO_2$ emissions from combustion devices can be reduced by improvements in energy conversion efficiencies. In conventional combustion devices, the chemical conversion of fuel and air into products occurs rapidly in an unrestrained and highly irreversible process (flame), with work extraction after the completion of combustion. This does not have to be the case. Conversion of fuel and air into products can be accomplished in a more reversible manner if the process is restrained so that work is extracted during the conversion process. An example of work extraction during fuel conversion is the fuel cell. What has not been previously recognized is that the fuel cell is not the only device that has this potential. Using high air preheat and dilute reactants, the chemical conversion process can be slowed to the point where mechanical energy extraction can be used to reduce the irreversibility of the energy conversion process and thereby increase efficiency. One example of controlled combustion is the well-known "flameless" oxidation process[1] in which exhaust heat recovery and exhaust gas recirculation are employed to cause combustion to occur in a more homogeneous fashion. An important additional benefit of this concept is that by controlling the peak temperature of the products, $NO_x$ emissions can be reduced by orders of magnitude over conventional combustion processes.

In the present project, this concept is being extended to include diluents such as nitrogen and carbon dioxide that could be produced in separation processes and delivered to the combustion system. Carbon dioxide is particularly interesting in that it can have both a thermal and chemical effect on the combustion reaction. The primary objective of the project is to develop and validate detailed models of the combustion chemistry for use in modeling low-irreversibility combustion engine concepts.

**Background:** Figure 1 shows the regimes of combustion processes in terms of the oxygen content of the oxidizer and the preheat temperature. The controlled combustion regime lies outside the regimes of conventional combustion processes as a result of the very low $O_2$ levels and high preheat temperatures, and the chemical processes in the controlled combustion regime are poorly understood at the fundamental level needed for design optimization, especially for high-pressure combustion systems, such as gas turbines and diesel engines.

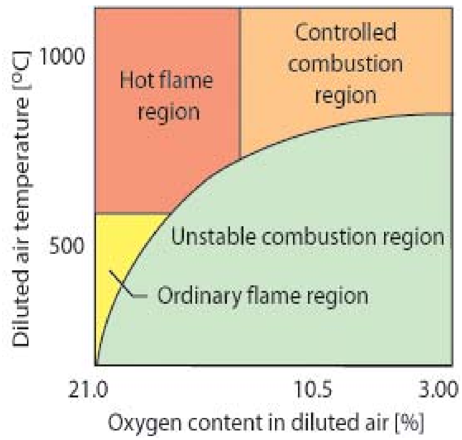


**Figure 1:** Regimes of combustion.

The regime of controlled combustion is being investigated experimentally in a high-pressure flow reactor facility, Fig. 2, in which important parameters, such as preheat and dilution can be independently controlled.

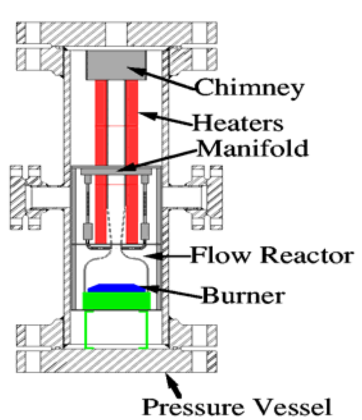


**Figure 2:** High-Pressure Flow Reactor (HPFR)

Figure 3 is a schematic layout of the reactor and the sampling instrumentation.

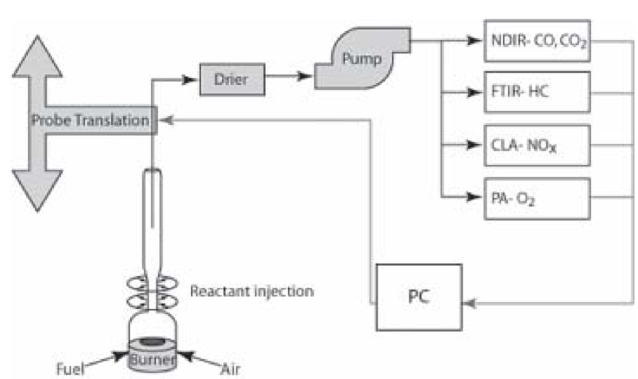


**Figure 3:** HPFR and sampling instrumentation.

The spatial evolution of the chemical reaction is monitored by sampling for key reactant, intermediate and product species using an extractive sampling probe coupled to on-line analyzers and temperature measured by a thermocouple probe. Detailed modeling of the profile data will yield chemical models for use in the design of controlled combustion systems and particularly for use in modeling low-irreversibility combustion engines, another project being carried out under the Global Climate and Energy Project[2]. The starting reaction mechanism is the Gas Research Institute mechanism, GRI-Mech 3.0, for natural gas combustion[3]. The fuels being used in the study include methane, ethane and methane-ethane mixtures (to simulate natural gas). The HPFR operates in the pressure range of 1-50 bar. Studies to date have been conducted at atmospheric pressure.

**Results**

Figure 4 show comparisons of calculated profiles of temperature, fuel, CO and $CO_2$ for methane and ethane at the nominal operating condition of the HPFR, which is in the controlled combustion regime shown in Fig. 1.

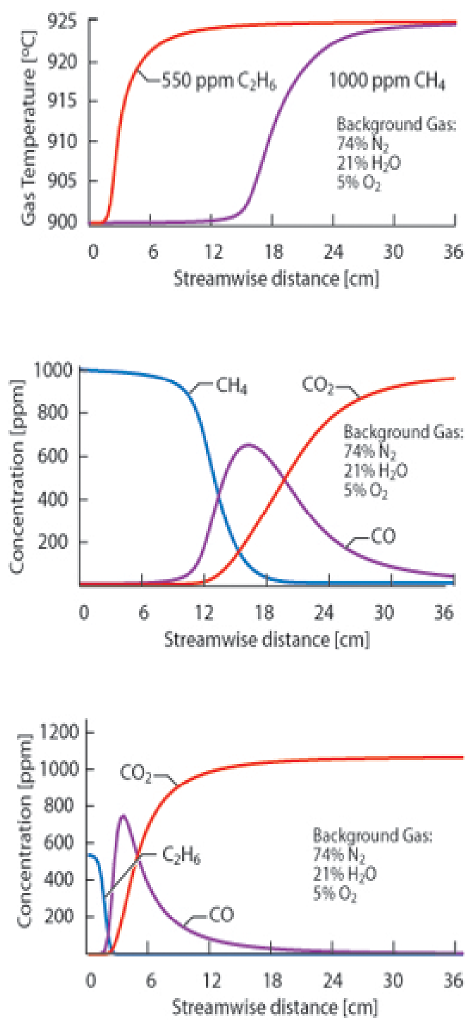


**Figure 4:** Temperature and species profiles for $CH_4$ and $C_2H_6$ for an initial mixture temperature of 900°C.

As expected, significant differences in fuel reactivity are observed at this operating condition.

Figure 5 shows initial comparisons of calculated and measured temperature profiles at atmospheric pressure for $CH_4$ and $C_2H_6$. Good agreement between the model predictions and the experimental data is found.

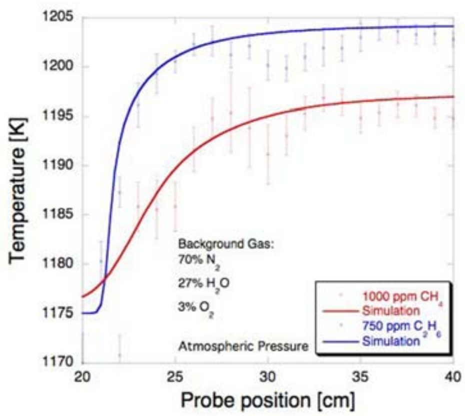


**Figure 5:** Comparison of calculated and measured temperature profiles for $CH_4$ and $C_2H_6$ at atmospheric pressure.

**Progress:** The majority of energy forecasts for the 21st century[4, 5] indicate increased use of fossil fuels to meet global energy demands, particularly in the transportation sector, with a corresponding increase in carbon emissions. Even the most optimistic forecasts[4] show significant dependence on fossil fuels for the first half of the century, with a leveling off of carbon emissions by mid century, but at levels that are higher than today. Hence, there can be a beneficial impact on carbon emissions by improvements in the energy conversion efficiencies of combustion-based power systems utilizing fossil fuels. Combining these higher efficiency systems with carbon capture could provide significant benefits in terms of reducing greenhouse gas emissions. The GCEP low-irreversibility combustion engine initiative, of which this project is a part, is investigating this novel approach to reducing irreversibilities through controlled heat release. Given the fundamental nature of this exploratory research effort, it is not possible to estimate the potential for reductions in emissions of greenhouse gases that result from energy use at this time.

**Future Plans:** Over the next year, experiments and modeling in $CH_4$-$C_2H_6$ systems will continue. Following completion of the atmospheric-pressure study, higher pressures will be investigated, starting initially at a pressure of 2 bar and then increasing pressure.

**References**

1. Tsuji, H. (ed), High Temperature Air Combustion: From Energy Conservation to Pollution Reduction, CRC Press, 2002.
2. Edwards, C. F., Low Irreversibility Combustion Engines, GCEP Advanced Combustion Project.

3. Smith, G. P., Golden, D.M., Frenklach, M. Moriarty, M.W., Eiteneer, B.,Goldenberg,M., Bowman, C. T., Hanson, R.K., Song, S., Gardiner, W.C., Lissianski, V.V., and Qin, Z. http://www.me.berkeley.edu/gri_mech/
4. Global Energy Perspectives, Cambridge University Press, 1998.
5. IEA Energy Outlook 2003, U.S. Department of Energy, 2003.


**Contact:** ctbowman@stanford.edu