COMBUSTION RESEARCH AND COMPUTER FLUID DYNAMICS

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Summary

Combustion engineers and researchers rely increasingly on mathematical modeling and numerical simulation for guidance in their analysis of combustion devices and designs for higher efficiencies and lower pollutant emissions. Laminar flame computer codes are available to compute the spatial distribution of temperature, gas and particle velocity and the concentrations of species. Current research is based on iterative comparisons between modeling and experiment, and allows for validating predictions derived from numerical computations. In the past only methods with intrusive probes were available, but today laser spectroscopic methods allow studying combustion details, such as free radical concentrations or soot formation without disturbing the reacting systems.

This chapter builds further on combustion and flame phenomena (see *Combustion Fundamentals*) and expands on the effects of turbulence in transport phenomena (see *Fundamentals of Transport Phenomena in Combustion*) and combustion research at large. Chemistry, combined with computer fluid dynamics, is considered in a few practical cases.

1. Combustion Research

1.1. Phenomena and Processes

Combustion seems a spontaneous and straightforward phenomenon, but in reality is extremely complex when it comes to the details of reaction chemistry and fluid dynamics. Some problems of tackling turbulence to treat heat and mass transfer problems are still largely unsolved. Moreover, integrating heat and mass transfer, reaction chemistry and fluid dynamics constitutes an extremely complex problem, involving:

- flow of combustion air, of fuels, and (after combustion) of flue gases, moved by both forced and induced draft in mutual balance to maintain the furnace under slight under-pressure,
- uniting gaseous, liquid, or solid fuels with combustion air, under suitable contact conditions, e.g. in co-current, counter-current, or cross-current flow,
- heating and ignition, followed by chemical reaction between fuels and combustion air,
- evolution of heat of combustion, and its spreading by radiation, convection, conduction, the balance being eventually carried along as sensible heat of hot flue gases,
- consecutive buoyancy of the combustion products.

Hence, combustion system may be considered from various viewpoints. An analytical approach requires adequate attention for each specific step, i.e.

1) **a chemical process**, proceeding by complex mechanisms composed of many thousands of elementary chemical steps involving short-lived intermediates, the free radicals. Elementary reactions proceed as actually written. Over-all combustion combines such elementary steps in reaction chains, in which

reactive intermediates carry the chain process, but no longer appear among the stable combustion products.

Each mechanism consists of elementary chemical reactions, each featuring its own reactants and products. These form or disappear in specific molar ratios fixed by stoichiometry, and determining the corresponding masses and volumes involved, as well as the amount of heat liberated. Remarkably, even the simplest combustion reactions, e.g. those of hydrogen, carbon monoxide, or methane take place through a multitude of elementary free radical reactions. Hence, describing kinetics and mechanism requires careful consideration of a large number of reactions (see *Combustion Fundamentals)*. Each has specific stoichiometry, reaction rate, heat of combustion, and chemical equilibrium. The latter two are fixed by concepts and data developed in chemical thermodynamics and thermochemistry, as explained further.

In most cases the complexity of the reacting system is ignored and only over-all stoichiometry, heat of reaction, and mass and heat balances are considered, greatly simplifying their study. Indeed, combustion reactions almost always seem instantaneous and rather complete: if it is mixed, it is burned! Still, it is sometimes necessary considering complex systems, to explain finer details of over-all reaction and kinetic behavior, e.g. the ignition delay, quenching and inhibition, and – in this context – the formation of pollutants, such as thermal, prompt, and fuel NO_x.

2) **fluid mechanics** is important from three different viewpoints:

- Natural or **mechanical draft** is required to supply fresh combustion air and eventually to evacuate the resulting products, either by natural draft (in small units, such as stoves), or by combined forced and induced draft (in industrial units). Forced draft refers to blowing in combustion air into the furnace, induced draft is aspiration created jointly by the stack and mechanically by an induced draft fan. A balance is struck between these two, since furnaces must operate under slight negative pressure, when compared to their surroundings, to prevent smoke and fumes from leaving through leaky locations. Both natural and chimney drafts derive from Archimedes' Law (see *Combustion Fundamentals*), which states that hot masses, lighter than the ambient air become buoyant and rise, leaving room for replacement by fresh air before combustion, or hot gases afterwards.
- Burners generate strongly non-isothermal, non-homogeneous reacting mixtures, with variable levels of turbulence and (possibly) induced swirl. Temperature differences, created by variable combustion rates, are somewhat equalized by fast radiant and convective heat transfer. Concentration differences of fuel and air and intermediate and final combustion products are rendered more uniform mainly by convective diffusion, molecular diffusion and heat conduction being comparatively slow. Laminar or transition flow applies only at a small-scale, such as the flame of a small Bunsen burner,
- Furnaces feature complex internal flow regimes, with specific recirculation and outflow patterns, related to furnace geometry and flow organization. For the sake of simplicity, plug or piston flow is postulated, assuming a constant residence time for all air and gas parcels. Lumped parameter or compartment

models consider mass balances only. Flow structure is described as piston flow, with or without axial dispersion. Experimental information is derived from tracer experiments. More sophisticated CFD-models accommodate various degrees of internal recirculation, short-circuiting of fluids and the presence of stagnant zones. Non-uniformities in the temperature, oxygen and residence time always have negative effects: part of the combustion products escapes early from the furnace, after a reduced residence time for combustion. Dead volumes formed by boundary layer separation and internal circulation eddies are characterized by low combustion rates, caused by low temperature and high conversion. Mixing reactants and introducing swirl are realized by well-located injection of high-velocity secondary air, as discussed further.

3) Heat transfer by conduction (mainly important at the walls of the furnace, or in solid or liquid fuel particles), convection, and radiation, from the high temperature combustion zones to heat sinks.

Incineration systems are often even more complex, given the heterogeneous and variable nature of waste and by erratic character of its combustion processes.

1.2. Combustion Conditions

The most important combustion conditions are summarized in Table 1.

Combustion Conditions	Combustion Temperature ° C	Furnace Temperature ° C	Gas Velocity $m\ s^{-1}$	Residence Time s	Air Number -	Thermal Volumetric Load MW m^{-3}	Thermal Cross-sectional Load MW m^{-2}
Power Plant							
Natural Gas	1100-1400	1000-1100	5-10	1-3	1.05-1.1	0.25-0.35	5-8
Oil	1100-1400	1000-1100	5-10	1-3	1.05-1.2	0.25-0.35	5-8
Grate stoker	1100-1300	1000-1100	4-9	1-3	1.3-2.5	0.15-0.35	0.5-2.5
Fluidized bubbling Bed Combustor	750-1050	750-1050	0.5-5	1-3	1.2-1.4	2-5	1-2
Circulating Fluid Bed Combustor	750-950	750-950	5-8	0.5-6	1.12-1.3	8-20	2-8
Pulverized coal firing	1100-1500	1050-1250	5-10	1-3	1.13-1.3	0.06-0.3	0.6-3
Pulverized lignite firing	1100-1300	950-1150	4-8	1-3	1.2-1.5	0.06-0.15	2.5-5
Pulverized coal firing (wet bottom)	1300-1600	1000-1150	5-10	1-3	1.15-1.3	0.1-0.4	4-6
Mechanical Grate MSW-Incinerator	1000-1250	1000-1100	3-8	3-6	1.5-2.0	0.15-0.35	1.4-1.6
Fluid Bed sludge Combustor	750-900				1.05-1.8	1-3	0.5-1

Stationary Combustion Chamber					1.2-3	0.1-0.3	0.1-1
Rotary Kiln Incinerator					1.6-3.5	0.15-0.2	1.5-2.5
Postcombustion Chamber	1050-1300	1050-1250			>1.4	0.08-0.35	1-1.5

Table 1: Combustion conditions

Combustion Temperature

The Combustion Temperature attained is basically a function of the liberated heat and the air number. The temperature is highest when the excess of air is nil or even negative, and descends according to a hyperbolic law when excess air is supplied.

A high Combustion Temperature leads to high reaction rates and fast heat transfer. However, it is also conducive to

- High NO_x.
- Building accretions on refractory by tacky ash.
- Refractory slagging.
- Volatilization of salts and heavy metals from ash. Eventually these condense to a hard-to-remove mist that either is emitted or requiring specialized abatement, such as wet electrostatic precipitators (see *Electrostatic Precipitators*).

Combustion temperatures are derived from the adiabatic flame temperature, reduced by an estimate, based on radiant heat losses.

Furnace Temperature

Furnace Temperature generally follows combustion temperature, but at a lower level, because of heat losses, post-combustion slower than flame combustion, and possibly – because of parasitic entrance of air, aspired into the combustion chamber by cracks, the slag extraction system, or other sources.

Furnace temperatures remain as a rule above 1000° C, with the single exception of fluid bed units, allowing a reasonably complete combustion to be attained below 900° C thanks to superior heat and mass transfer characteristics. The tackiness of ash or of neutralization salts may impede operation at conventional temperatures.

Some fluid bed combustors even operate between 450 and 600° C, in a gasification mode, with combustion completed in the freeboard zone (see *Waste Incineration Technology*). Such temperatures are suitable for controlling combustion when high calorific waste, e.g. automobile shredder residue, is fired.

Gas Velocity

A high gas velocity is often desirable, since convective heat transfer is promoted, the Nusselt-number varying more or less with the Reynolds Number as $Re^{0.7}$ (see

Fundamentals of Transport Phenomena in Combustion). However, there are good reasons for limiting the gas flow to some 10 m s^{-1}, namely:

- Pressure drop is proportional to flow rates to a power between 1 and 2. Hence, there is an economic optimum between productivity (more gas flowing through the plant) and operating cost (draft requirements, the main consumer of electric power in a plant).
- Erosion becomes problematic at linear velocities of ca. 10-15 m s^{-1}.
- Fouling of heat exchanger surfaces is strongly enhanced by inertial deposition of tacky fly-ash particles. For that reason in incinerators the gases must be cooled in empty radiant boiler flues down to a temperature at which fly-ash is no longer tacky.

Residence Time

A Residence Time of 1-3 seconds is sufficient for attaining acceptable levels of combustion. Gas and oil are much faster to burn than solid fuels, also after adequate pulverization.

Air Number

Gaseous fuels can be fired under almost stoichiometric conditions. Liquids, depending on their viscosity and the burner design, require a somewhat larger excess, whereas solid fuel stokers demand a sizeable air number. The excess requirements are reduced by better pre-mixing and improving the mixing conditions induced by secondary air.

Thermal Volumetric Load

The Thermal Volumetric Load mainly varies with the intensity of combustion. Compared to gas or oil, the load is rather limited when firing coal or lignite. Rotary kilns offer only low Thermal Volumetric Loads, whereas those in fluidized bed units are exceptionally high, as are the internal and external (to the wall, if this is a boiler membrane) rates of heat transfer. This also explains the development of pressurized fluid bed units, since these attain still higher rates, allowing a compact and less expensive design. The latter is essential, since – on the basis of strength considerations the reactor wall is proportional to both diameter and pressure level.

The thermal load factors are all resulting from empirical observations. A logical basis can be provided by the analytical methods, applied in computer fluid dynamics. Traditionally, Thermal Volumetric Load and capacity values are given on a basis of Gcal m^{-3} h^{-1} and Gcal h^{-1}. Today, these have to be replaced by MW m^{-3} (= MJ m^{-3} s^{-1}).

2. Combustion Research

2.1. Survey

Combustion Research was originally directed towards **fluid mechanics,** combined with the thermal balance, including the release of heat of combustion. A usual simplifying assumption was to postulate that combustion proceeds infinitely fast. This approach copes well with designing and modeling stationary combustion processes, but becomes inadequate when tackling transient processes, such as **ignition, quenching**, or studying the formation of particular pollutants, closely related to flame and post-flame phenomena, such as CO, or NO.

For these problems the coupling of the fluid flow equations and the chemical reaction terms is essential. At the fluid mechanics side, there is the turbulence generated by heat release, and the turbulent flow confronted with density changes as typical problems. The chemical reaction proper is characterized by very extensive reaction mechanisms, totaling hundreds of elementary reactions. Of course, a simplified approach remains possible.

In a **chemically reacting flow** the system at each point in space and time is completely described by specifying:

- Temperature, pressure, density,
- The flow velocity, and
- The concentration of each species.

These properties can change in space, as a result of fluid flow (convection), molecular transport (heat conduction, diffusion, viscosity), radiation, and chemical reaction. They may also change in time, under non-stationary flow or combustion conditions. A mathematical description of flames and combustion has to account for each of these processes.

Mass, energy, and momentum all are conserved in reacting flows. The conservation equations, also termed **equations of change**, describe the reacting flow, by summation of these conserved properties over all relevant processes (cf. *Fundamentals of Transport Phenomena in Combustion*). Since all systems are described by the same equations the main differences are to be found in geometrical features and boundary conditions of the system, and in physicochemical conditions and flow characteristics, characterized by a series of dimensionless numbers related to:

- Flow (**Reynolds** Number),
- Physical properties (**Prandtl** and **Schmidt** Numbers),
- The effect of gravity (**Froude** Number; *Fr*), etc.

Many more dimensionless numbers have been introduced, in relation to specialized studies, e.g. of atomizing and burning oil turbulence.

Important aspects of combustion research deal with:

- measurement of physical factors, such as temperature and pressure in the combustion chamber, velocity, density, concentration, and particle sizes,
- thermodynamics,

- transport phenomena (see *Fundamentals of Transport Phenomena in Combustion*),
- chemical kinetics and reaction mechanisms (see *Combustion Fundamentals*),
- the Navier-Stokes equations,
- the basic flame types, i.e. premixed and non-premixed laminar and turbulent flames (see *Combustion Fundamentals*),
- combustion of liquid and solid fuels, their ignition and low temperature oxidation, engine knock, and finally (see *Combustion Fundamentals*),
- environmental issues, with special interest for the formation of nitric oxides, hydrocarbons, and soot (see *Control of Sulfur Oxides* and *Thermal and Catalytic Combustion*).

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Biographical Sketch

Alfons Buekens was born in Aalst, Belgium; he obtained his M.Sc. (1964) and his Ph.D (1967) at Ghent University (RUG) and received the K.V.I.V.-Award (1965), the Robert De Keyser Award (Belgian Shell Co., 1968), the Körber Foundation Award (1988) and the Coca Cola Foundation Award (1989). Dr. Buekens was full professor at the Vrije Universiteit Brussel (VUB), since 2002 emeritus. He lectured in Ankara, Cochabamba, Delft, Essen, Sofia, Surabaya, and was in 2002 and 2003 Invited Professor at the Tohoku University of Sendai.

Since 1976 he acted as an Environmental Consultant for the European Union, for UNIDO and WHO and as an Advisor to Forschungszentrum Karlsruhe, T.N.O. and VITO. For 25 years, he advised the major industrial Belgian Bank and conducted more than 600 audits of enterprise.

Main activities are in thermal and catalytic processes, waste management, and flue gas cleaning, with emphasis on heavy metals, dioxins, and other semi-volatiles. He coordinated diverse national and international research projects (Acronyms Cycleplast, Upcycle, and Minidip). Dr. Buekens is author of one book, edited several books and a Technical Encyclopedia and authored more than 90 scientific publications in refereed journals and more than 150 presentations at international congresses. He is a member of Editorial Boards for different journals and book series.

He played a role in the foundation of the Flemish Waste Management Authority O.V.A.M., of a hazardous waste enterprise INDAVER, and the Environmental Protection Agency B.I.M./I.B.G.E. He was principal ministerial advisor in Brussels for matters regarding Environment, Housing, and Classified Enterprise (1989). Since 1970 he has been a Member of the Board of the Belgian Consumer Association and of Conseur, grouping more than a million members in Belgium, Italy, Portugal, and Spain.

He is licensed expert for conducting Environmental Impact Assessments (Air, Water, Soil) and Safety Studies regarding large accidents (Seveso Directive).