

# CHEMICAL KINETICS FOR COMBUSTION

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## 1. INTRODUCTION

The quantitative description and understanding of combustion processes needs extreme computational efforts and has at present to be restricted to relatively simple cases, due to a very complex interaction of chemical reaction, transport, and convection described by instationary or stationary partial differential equation systems.

However, even a rather simplified treatment can give a lot of insight into combustion processes, as demonstrated in the following mainly for 1D and 2D systems. Typical combustion processes are considered in the following with emphasis on three topics:

1. *Basic Physics and Chemistry of Combustion Processes; Homogeneous Reaction Systems:* Processes like transport phenomena (heat conduction, mass diffusion etc.), thermodynamics, and chemistry in spatially homogeneous systems are studied because of their importance as basic elements of simple combustion processes.
2. *Structure of Laminar Flame Fronts; Stationary and Instationary Flame Propagation:* Premixed and diffusion flame fronts are basic elements of turbulent flames in cases where chemical reaction can be assumed to take place in relatively thin layers ("*flamelet model*"). The structure of stationary laminar flame fronts as the result of the interaction of transport, chemistry, and flow is considered in detail for simple hydrocarbon fuels. Instationary behaviour plays an important role in ignition processes and for phenomena like quenching of turbulent flames, noise generation, etc.
3. *Pollutant Formation Chemistry; Consequences for Turbulent Combustion:* A detailed description of the chemistry of combustion is necessary to describe and understand pollutant formation (nitrogen oxides, polycyclic hydrocarbons, soot, etc.). Different methods are described to include detailed chemistry in terms of sets of elementary reactions into turbulent combustion modelling.

## 2. BASIC PHYSICAL CHEMISTRY OF COMBUSTION PROCESSES

### 2.1 Thermodynamic Data

Thermodynamic data are needed to calculate specific heat capacities and enthalpies in the energy balance equation and for the computation of reverse reaction rate coefficients in the reaction mechanism (see below). For this purpose, polynomial fits of species molar heat capacities  $C_{p,i}$  are used, consisting of seven coefficients for high ( $T > 1000$  K) and low ( $T < 1000$  K) temperature (in each case five coefficients for molar heat capacities  $C_{p,i}$ , and two integration constants for enthalpy and entropy; details in [1, 2]). Examples are given in Table 1.

*Table 1: Examples for Polynomial Representation of Thermodynamic Data*

O	J 3/770	100	000	000	OG	300.000	5000.000		1
	0.25342961E+01	-0.12478170E-04	-0.12562724E-07	0.69029862E-11	-0.63797095E-15				2
	0.29231108E+05	0.49628591E+01	0.30309401E+01	-0.22525853E-02	0.39824540E-05				3
	-0.32604921E-08	0.10152035E-11	0.29136526E+05	0.26099342E+01					4
O2	J 3/770	20	00	00	OG	300.000	5000.000		1
	0.36122139E+01	0.74853166E-03	-0.19820647E-06	0.33749008E-10	-0.23907374E-14				2
	-0.11978151E+04	0.36703307E+01	0.37837135E+01	-0.30233634E-02	0.99492751E-05				3
	-0.98189101E-08	0.33031825E-11	-0.10638107E+04	0.36416345E+01					4
N	J 6/770	1N	10	00	OG	300.000	5000.000		1
	0.28897814E+01	0.10005879E-02	-0.22048807E-06	0.20191288E-10	-0.39409831E-15				2
	0.38857042E+04	0.55566427E+01	0.38737300E+01	-0.13393772E-02	0.16348351E-05				3
	-0.52133639E-09	0.41826974E-13	0.35802348E+04	0.34202406E+00					4
N2	J 3/77N	2N	00	00	OG	300.000	5000.000		1
	0.28532899E+01	0.16022128E-02	-0.62936893E-06	0.11441022E-09	-0.78057465E-14				2
	-0.89008093E+03	0.63964897E+01	0.37044177E+01	-0.14218753E-02	0.28670392E-05				3
	-0.12028885E-08	-0.13954677E-13	-0.10640795E+04	0.22336285E+01					4
CHO	J12/70H	1C	10	10	OG	300.000	5000.000		1
	0.34738348E+01	0.34370227E-02	-0.13632664E-05	0.24928645E-09	-0.17044331E-13				2
	0.39594005E+04	0.60453340E+01	0.38840192E+01	-0.82974448E-03	0.77900809E-05				3
	-0.70616962E-08	0.19971730E-11	0.40563860E+04	0.48354133E+01					4
CH2	J12/72C	1H	2	0	OG	300.000	5000.000		1
	0.30643921E 01	0.33640424E-02	-0.10989143E-05	0.15985906E-09	-0.84323282E-14				2
	0.45435059E 05	0.49476233E 01	0.36884661E 01	0.14331874E-02	0.57268682E-06				3
	-0.99654077E-10	-0.11374164E-12	0.45305152E 05	0.18445559E 01					4
CH3	T11/79C	1H	3	0	OG	300.000	5000.000		1
	0.32985334E 01	0.51838532E-02	-0.15955029E-05	0.21366862E-09	-0.99468265E-14				2
	0.16425031E 05	0.29979439E 01	0.35155468E 01	0.34882184E-02	0.18435312E-05				3
	-0.27320166E-08	0.97533353E-12	0.16448859E 05	0.22105637E 01					4

Mixture specific enthalpies  $h$  and mixture specific heat capacities  $c_p$  are then determined from arithmetic means using the mass fractions  $w_i$  as weight:

$$c_p = \sum_i w_i c_{pi} \quad ; \quad h = \sum_i w_i h_i$$

### 2.2 Transport Models

Diffusive processes take care of broadening of steep profiles, where the temporal change of the quantity considered (e. g. temperature  $T$ , mass fractions  $w_i$ , velocity  $v$ , ...) are proportional to the curvature of the actual profile (2nd law of Fourier for  $T$ , 2nd law of Fick for  $w_i$ ,  $z$  is the space coordinate):