Exam topics to course
“The chemistry and physics of flames”

1 Basic notions of combustion science

What is combustion and what is a flame? Typical combustion reactions. Main types of flames. Features of laminar / turbulent and premixed / non-premixed flames. The Hindenburg disaster. Equivalence ratio. Definition and typical magnitude of laminar flame velocity. The change of laminar flame velocity with equivalence ratio, pressure and initial temperature.

2 The flame of a candle

The chemistry and physics of a candle flame. Evaporation and pyrolysis of the paraffin. The change of equivalence ratio inside the candle flame. Why is the candle flame yellow? The shape of the flame at normal gravity (1 g) and in microgravity. Investigation of flames at zero gravity or microgravity.

3 The combustion of hydrogen

The overall chemical equation and the 10-step mechanism. The change of explosion limits with temperature and pressure. Explanation to the explosion limits. The effect of heterogeneous reactions. The change of the branching ratio of reaction step $H+O_2 \rightarrow$ with pressure, temperature and gas composition. Spread of the hydrogen–air flame.

4 Combustion of wet CO, methane and other alkanes

The significance of syngas in environmental protection. Reaction steps of wet CO combustion. C1 and C2 reaction chains of methane combustion. The reaction steps of the C1 and C2 chains. Combustion of higher alkanes (ethane, propane, buthane). Why is the flame of hydrocarbons blue?

5 Internal combustion engines

The operation of Otto- and Diesel-engines. HCCI-engine, stratified charge engines. The advantages and disadvantages of the various types. The aspect of environmental protection. Change of pressure in the cylinder of a petrol engine during normal operation and knocking. What is knocking? Determination of the knocking properties of fuels. RON, MON and PON.

6 Low-temperature hydrocarbon oxidation

Chain branching mechanism below 900 K. The reaction steps of low temperature propane oxidation. The characteristic features of intramolecular hydrogen abstraction. Why does the knocking depend on the structure of the fuel molecule? The HO_2/H_2O_2 explosion route. Two stage ignition, negative temperature coefficient (NTC) ignition and cool flames.

7 Production of nitrogen oxides in combustion

Pollutant formation during combustion. The main routes of NO formation: thermal NO (or Zeldovich NO), prompt NO (or Fenimore NO), NO generated via N_2O, NO generated via NNH, and NO generated from fuel-bounded nitrogen. The chemistry of the various routes and their features.

8 Methods for decreasing NO emission

Primarily and secondary methods and their features. The chemistry of staged combustion and reburn. Selective catalytic reduction: Thermal DeNOx, RaPreNOx and NOxOut processes. The usage of AdBlue.

9 Soot

Advantages and disadvantages of soot formation. The process of soot formation. PAH. The HACA mechanism. Soot and the global warming.

10 Heterogeneous ignition and combustion

Sticking coefficient and surface coverage. What is happening with the H_2 and O_2 molecules on a Pt surface? $H_2/O_2/Pt$ reaction: the shift from slow surface reaction to gas phase flame propagation by increasing the temperature. Experimental investigation of heterogeneous ignition. Why is the heterogeneous ignition temperature increasing by increasing the concentration of CO or H_2? Why is the heterogeneous ignition temperature decreasing by increasing the concentration of CH_4 or C_2H_6 ? Applications of heterogeneous combustion. Three-way car catalysts.

11 Reaction kinetics and thermodynamic data in a detailed combustion mechanism
Temperature dependence of the thermodynamic data. Temperature dependence of the rate coefficient: Arrhenius equation and the extended Arrhenius equation. Pressure dependence of the rate coefficients: unimolecular decomposition and complex-forming bimolecular reactions. Lindemann model, Troe parameterization. The shape of the fall-off curve. Concentration units and their features. Calculation of temperature change in homogeneous reaction mixtures. CHEMKIN simulation codes and the CHEMKIN mechanism format.

12 Indirect measurements 1: Measurement of ignition delay time and concentrations
Measurement of ignition delay times in shock tubes and rapid compression machines. The limitations of the measurements. Measurement of concentrations coupled with the following types of reactors: perfectly stirred reactor (PSR), tubular reactor, shock tube.

13 Indirect measurements 2: Measuring the laminar flame velocity
Flame propagation in a tube, flame cone method, outwardly propagating spherical flame, twinflame method, heat flux burner method.

14 Direct measurements 1: Using lasers for the production and detection of radicals
Why are the radical–molecule and radical–radical reactions so important? The principles of lasers. Common lasers used in gas kinetics: excimer laser, Nd-YAG laser, dye laser. Applications of lasers for generating radicals and measuring the concentrations of radicals with laser induced fluorescence (LIF). Measuring light intensity with a photomultiplyer.

15 Direct measurements 2: Slow flow reactor with pulsed laser photolysis (PLP) and laser induced fluorescence (LIF) detection
Direct measurement with pulsed laser photolysis (PLP) radical generation and laser induced fluorescence (LIF) radical detection. The layout of the PLP-LIF apparatus. Application for a given elementary reaction. Features of the PLP-LIF method.

16 Direct measurements 3: Methods for the measurement of radical concentrations
Laser induced fluorescence (LIF), resonance fluorescence (RF), atomic resonance absorption spectroscopy (ARAS), light absorption, mass spectrometry, synchrotron vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS).

17 Direct measurements 4: Methods for the generation of radicals
Traditional flash photolysis, pulsed laser photolysis (PLP), discharge flow, shock tube.

18 Uncertainty of data
Uncertainty of data used in combustion modelling. Why is the quantitative modelling of combustion systems possible? Multichannel reactions. NIST Chemical Kinetics Database. Uncertainty of rate parameters, uncertainty of the enthalpies of formation, typical uncertainty of experimental data.

19 Databases of combustion measurements and validation of reaction mechanisms
The earlier databases (CloudFlame, RCM database, ChemKED, PrIMe)
ReSpecTh information site / Re branch (indirect and direct measurements, programs, mechanisms)
testing or reaction mechanisms („validation”)
plots of measured data points and simulation results, E error function values, and stacked bars

20 Reactive flows and the simulation of flames
Reactive flows. The properties of a flow and the effects that change these properties. Computational Fluid Dynamics (CFD). Simplifying assumptions for the description of 1D flames. The general 1D balance equation for conserved property E. The meaning and dimension of each quantity. The simplifying assumptions of Frank-Kamenetskii. The two-variate equation and its conversion to a single variate differential equation. Lewis number. Dependence of the flame velocity on the diffusion constant and the rate of the chemical reaction.