Exam topics for the course
"Analysis of kinetic reaction mechanisms"

1. **Reaction kinetics basics**
   stoichiometric equation, reaction mechanism, parameterization of temperature dependence, stoichiometric matrix, calculation of **J** and **F** matrices, general characteristics of the system of kinetic differential equations, trajectories, conserved properties; reaction kinetic simplifying principles: rate determining step, quasi steady state approximation (QSSA), fast pre-equilibrium approximation, pool component approximation; applications of reaction kinetics models

2. **Construction of detailed reaction mechanisms and the reaction pathways**
   data sources, traditional construction of reaction mechanisms, automatic mechanism generation; pathway analysis: species conversion pathways, element following pathways, pathways leading to the production of a given species

3. **Local sensitivity analysis 1**
   local sensitivity coefficient and its interpretation, system of differential equations for local sensitivity coefficients, initial concentration sensitivity coefficients, calculation of sensitivity coefficients with finite difference approximation, calculation of sensitivity coefficients with the Direct Method and the Decoupled Direct Method, automatic differentiation

4. **Local sensitivity analysis 2**
   original and normalized sensitivities, principal component analysis of the sensitivity matrix, local uncertainty analysis, applications of local sensitivities

5. **Global uncertainty analysis and global sensitivity analysis**
   local and global uncertainty analysis. Morris' screening method, Monte Carlo method, Latin hypercube sampling, Fourier Amplitude Sensitivity Test (FAST) method, sensitivity indices, surface response methods, polynomial chaos expansion (PCE) method, high-dimensional model representation (HDMR) method.
   What is uncertainty analysis generally good for?

6. **Uncertainty of the thermodynamic and kinetic parameters**
   uncertainty of thermodynamic data, Active Thermochemical Tables (ATcT), direct and indirect measurements, estimation of uncertainty for gas kinetic rate coefficients, EXAMPLE: applications of several uncertainty analysis methods to a methane flame model

7. **Uncertainty of the Arrhenius parameters**
   temperature dependence of uncertainty factor *f*, domain of uncertainty of the Arrhenius parameters, joint uncertainty of the Arrhenius parameters, calculation of the covariance matrix of the Arrhenius parameters, determination of the covariance matrix of the Arrhenius parameters from literature measurements

8. **Mechanism optimisation and determination of the posterior parameter uncertainties**
   steps of mechanism optimisation, relations between the following uncertainty domains: prior uncertainty of the input parameters, uncertainty of the model results calculated from the prior uncertainty of the input parameters, uncertainty of model results measured by indirect experiments, prior uncertainty of the input parameters, uncertainty of the model results calculated from the posterior uncertainty of the input parameters; results of mechanism optimization

9. **Time-scale analysis**
   lifetime and its interpretation for various systems, stiff systems, slow and fast variables, slow manifolds in dynamical systems, modes, calculation of the dynamical dimension, stability analysis of stationary and dynamic systems

10. **Reduction of reaction mechanisms 1: Elimination of redundant reactions**
    General principles, characteristics of detailed mechanisms. Why is it permitted and useful to reduce reaction mechanisms? Rate-of-production analysis, principal component analysis of matrices **S** and **F**, integer programming methods, genetic algorithm-based methods.

11. **Reduction of reaction mechanisms 2: Elimination of redundant species**
    Reaction rate and Jacobian-based methods for species removal, species elimination via trial and error, connectivity method (CM), simulation error minimization connectivity method (SEM-CM)
    directed relation graph (DRG) method, DRG-aided sensitivity analysis (DRG-SA),
    DRG with error propagation (DRGEP), path flux analysis method (PFA),
    comparison of methods for species elimination

12. **Reduction of reaction mechanisms 3: Lumping**
    reaction lumping; species lumping: linear lumping, general nonlinear methods, chemical lumping, continuous lumping

13. **Reduction of reaction mechanisms 4: Time scales**
    history of the quasi steady-state approximation, calculation of the local QSSA error, interpretation of QSSA, Computational Singular Perturbation (CSP), reduction of models in reaction kinetics with direct calculation of slow manifolds (ILDM), reaction diffusion manifolds (REDIM), repro-modelling

14. **Computer codes for the study of complex reaction systems**
    general simulation codes in reaction kinetics, simulation of gas kinetics systems, analysis of reaction mechanisms, investigation of biological reaction kinetic systems, codes for global uncertainty analysis, ReSpecTh Information Site