A Tribute to Juergen Warnatz

Prof. Dr. Frank Behrendt
Technical University of Berlin

The World of Reactive Flows …

- **Heidelberg 1982 - 1988**
- **Stuttgart 1989 - 1994**
- **Heidelberg 1995 - 2007**

… with Jürgen Warnatz leading from the front

Awards

- 1981 - Karl-Winnacker-Award (DM 50.000,--)
- 1982 - Silver Combustion Medal
- 1991 - Philip-Morris Research Award (DM 30.000,--)
- 1993 - Gottfried-Wilhelm-Leibniz Award (DM 1.500.000,--)
- 1994 - Gerhard-Damköhler-Medal
- 1996 - Russel Severance Springer Professor, UC Berkeley
- 1997 - Dr. techn. h. c., Universitetet Trondheim, Norway
- 2001 - A. K. Oppenheim Prize
- 2005 - Visiting Professor, Stanford University

A Physicist Finding His Way

… from Darmstadt

… with a detour
via Livermore

… to Heidelberg

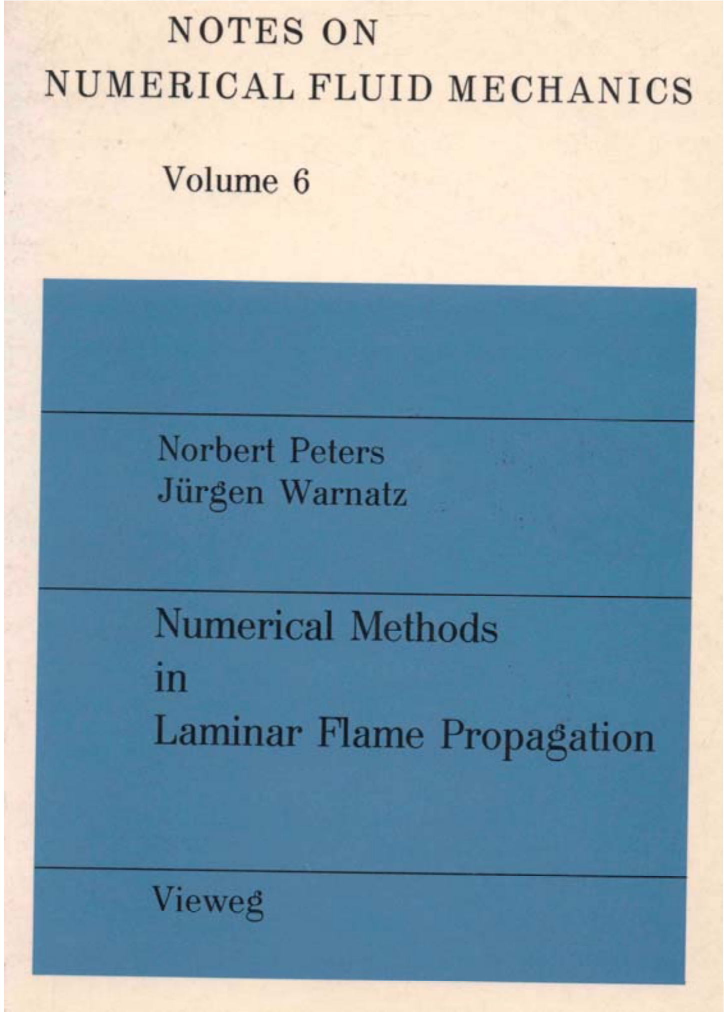
First Steps in Heidelberg: 1982 - 1988

- **SFB 123 - Stochastische Mathematische Modelle**
  - **Laminar premixed flames**
  - **Counterflow non-premixed flames**
  - **Homogeneous ignition processes**
  - **Instationary Flames**

… and all with detailed reaction mechanisms for various fuels

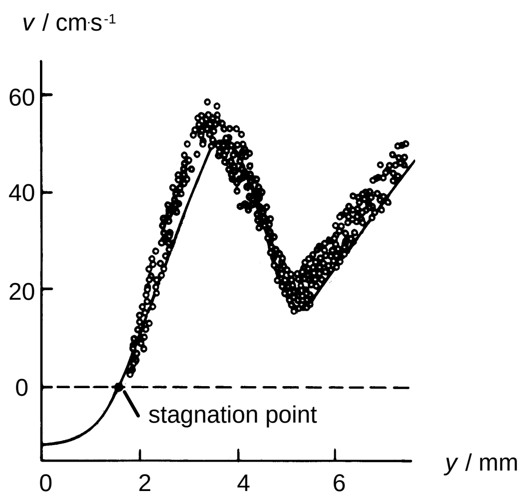
Heidelberg
- Laminar Premixed Flames

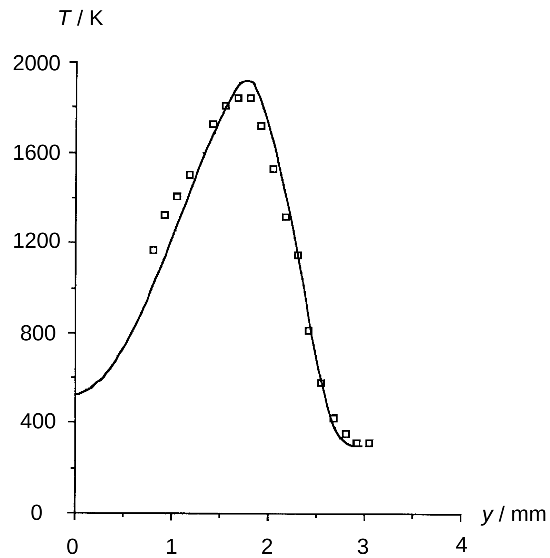
- **Based on a workshop organized by N. Peters and J. Warnatz in Aachen 1981**
- **Two problems are addressed:**
  - **1D laminar flames with 1-step-kinetics**
  - **1D laminar flames with detailed kinetics**

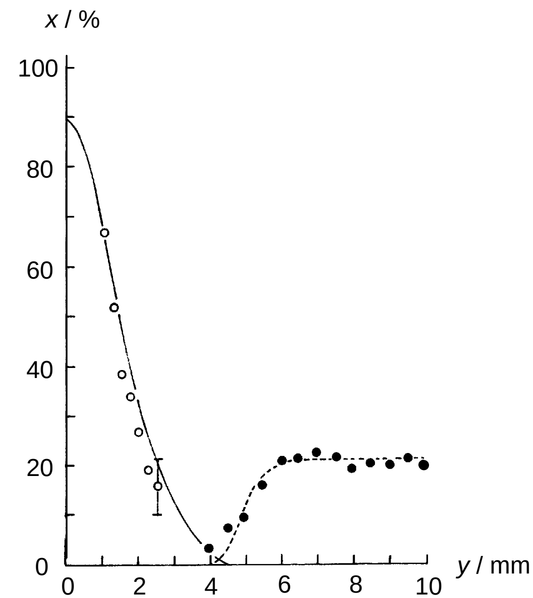


Heidelberg
- Counterflow Non-Premixed Flames

Building Block for Flamelet Model of Turbulent Combustion (B. Rogg)

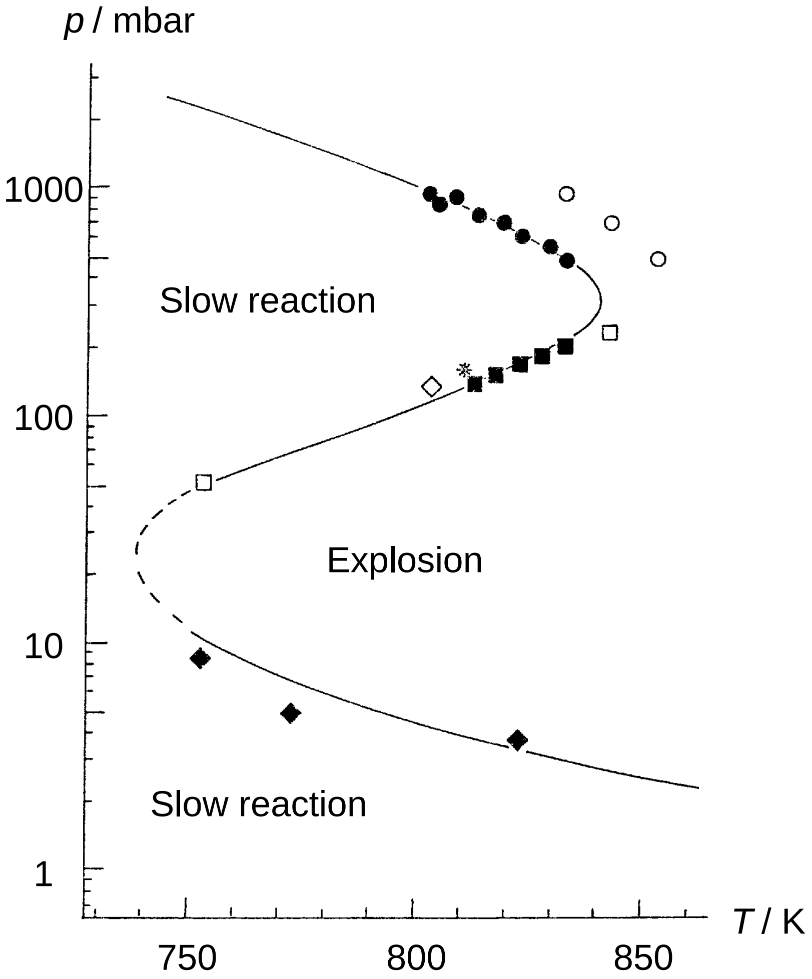






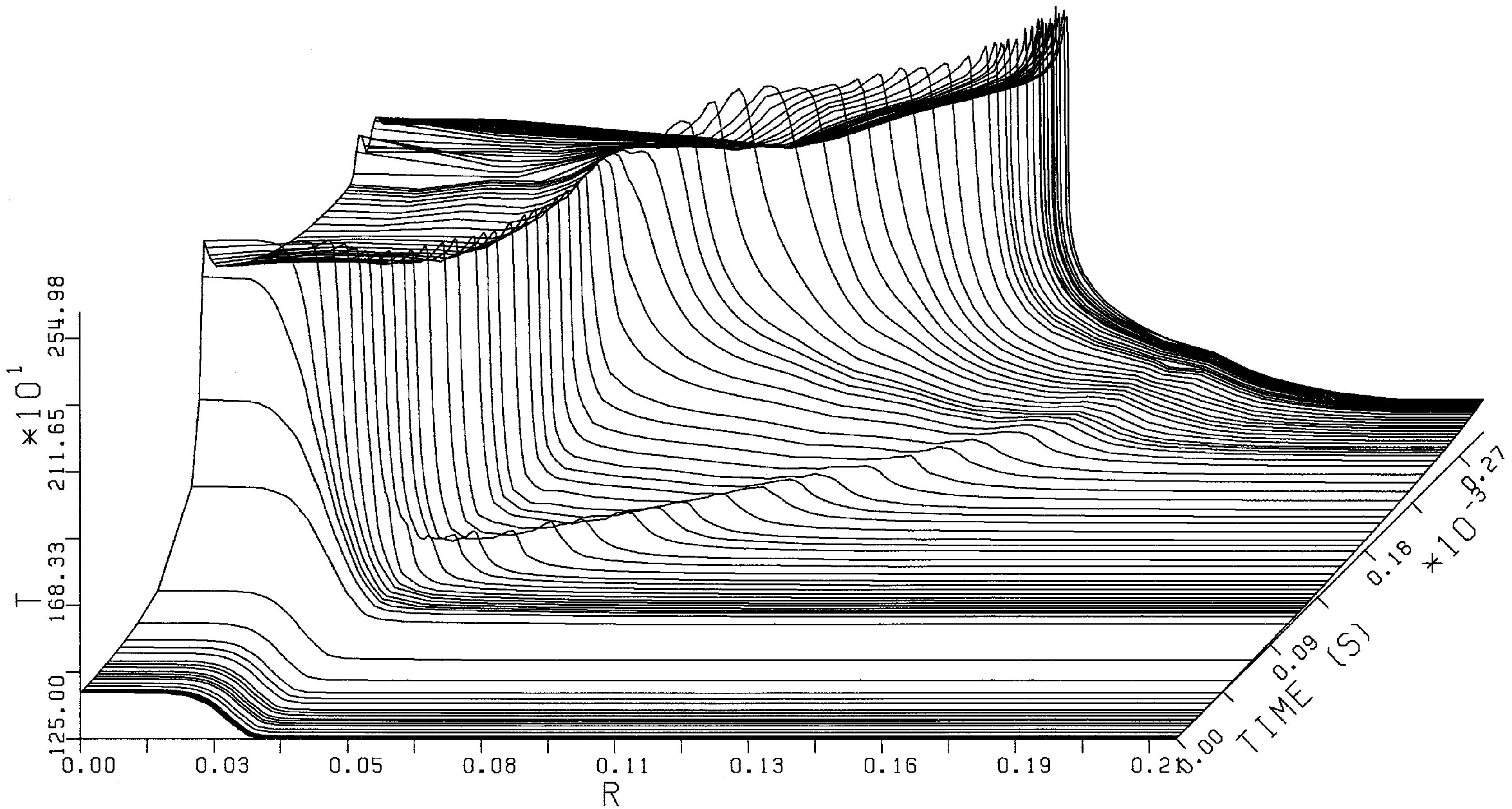
G. Dixon-Lewis, T. David, P. H. Gaskell, S. Fukutani, H. Jinno,
J. A. Miller, R.J. Kee, M.D. Smooke, N. Peters, E. Effelsberg, F. Behrendt, J. Warnatz
Calculation of the Structure and Extinction Limit of a Methane-Air Counterflow Diffusion Flame in the Forward Stagnation Region of a Porous Cylinder.
PCI **20**, 1893-1904 (1985).

Heidelberg
- Homogeneous Ignition Processes



U. Maas

Heidelberg
- Instationary Flames



G. Goyal, U. Maas

Teaming-up with Engineers in Stuttgart

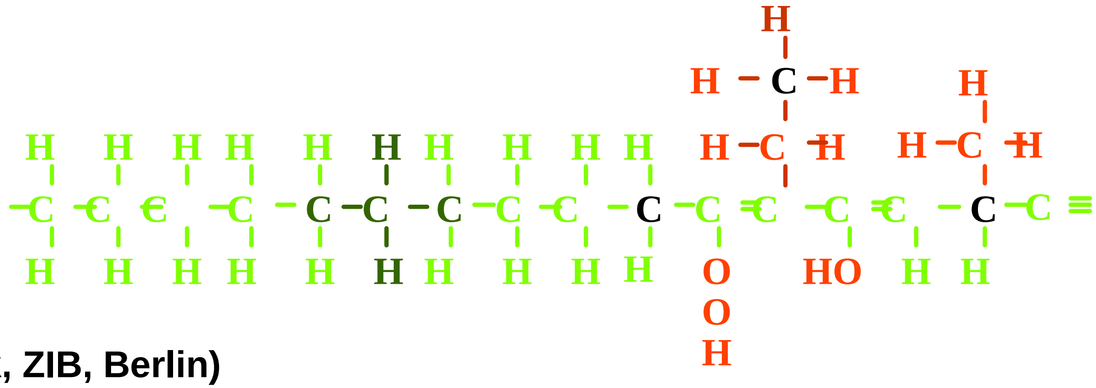
- Automatic generation of reaction mechanisms
- Low temperature ignition
- How does an engine knock?
- Hermes did fly nicely in simulations
- First step into the field of heterogeneous reactions

Stuttgart
- Automatic Generation of Reaction Mechanisms

The dream of a kineticist

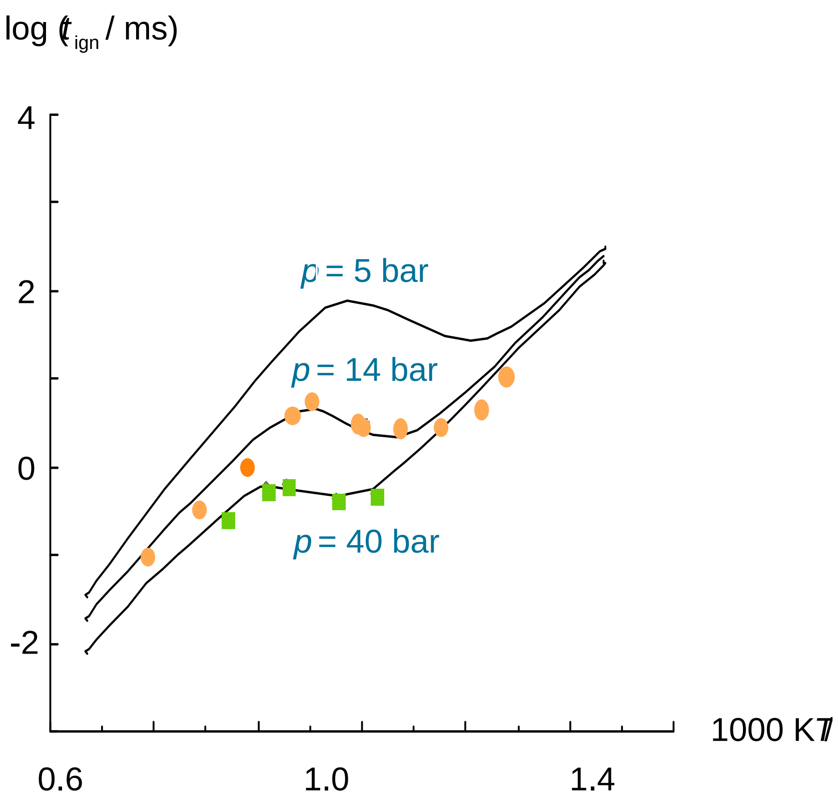
- Automatic generation of an detailed reaction mechanism of elementary reaktions
- Automatic reduction to a specified number of global reactions

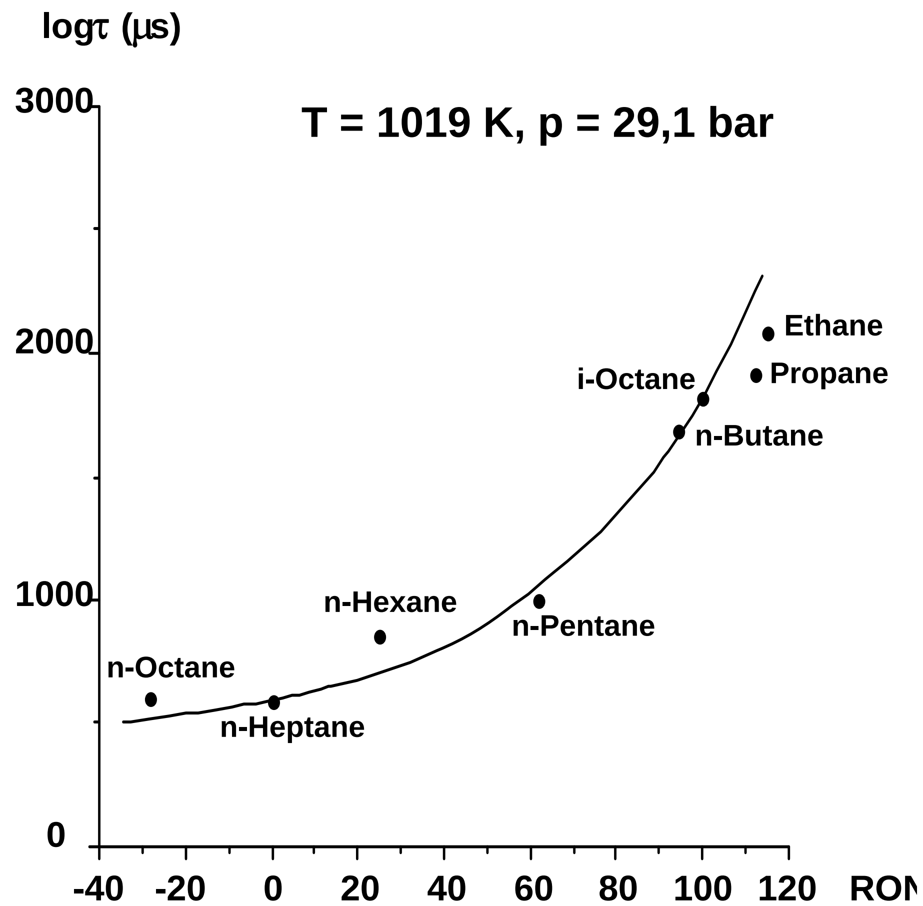
First steps to realize this dream by programming a LISP code generating mechanism based on rule sets



(Cooperation with H. Melenk, ZIB, Berlin)

Stuttgart
- Low-Temperature Ignition

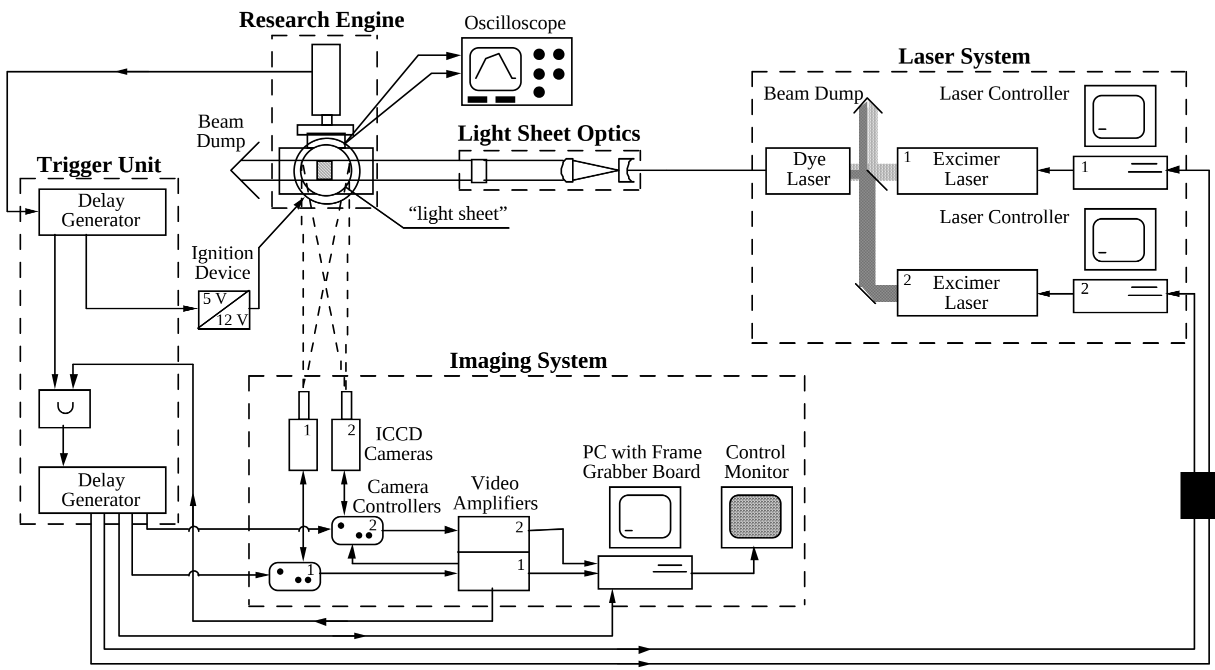


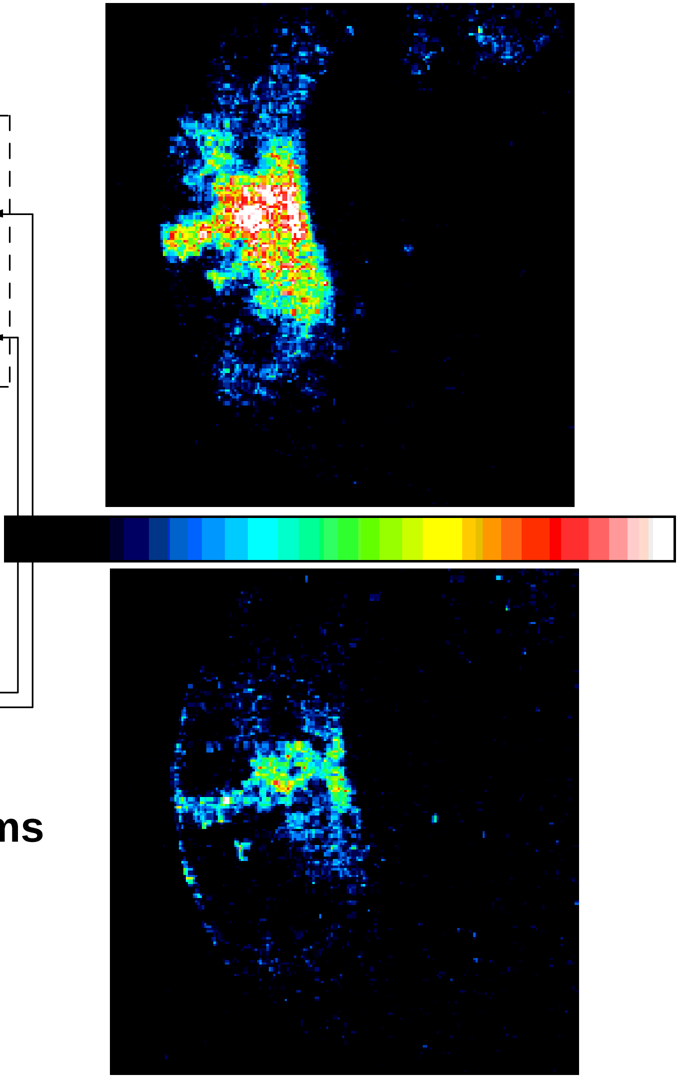


Experimental data by Adomeit et al.

C. Chevalier, C. Esser

Stuttgart
- How does an Engine Knock?



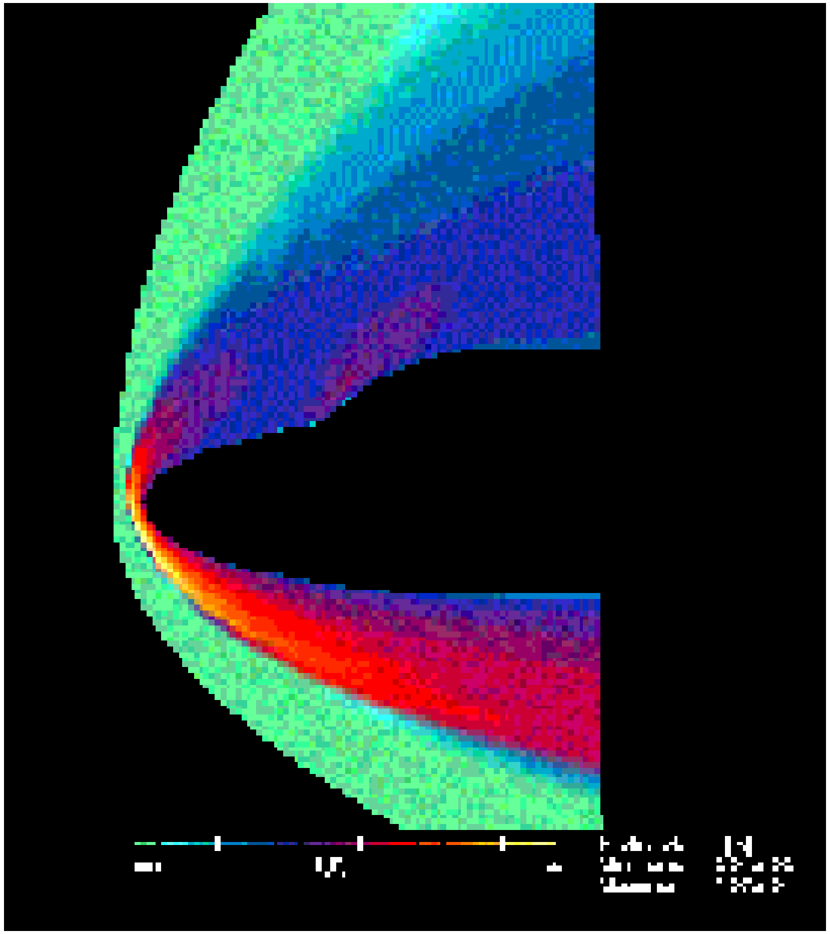


PRF 90, 1000 1/s, Ign. 16 deg BTDC
upper picture: 9,6 deg ATDC, lower picture: +0,15 deg/25 ms

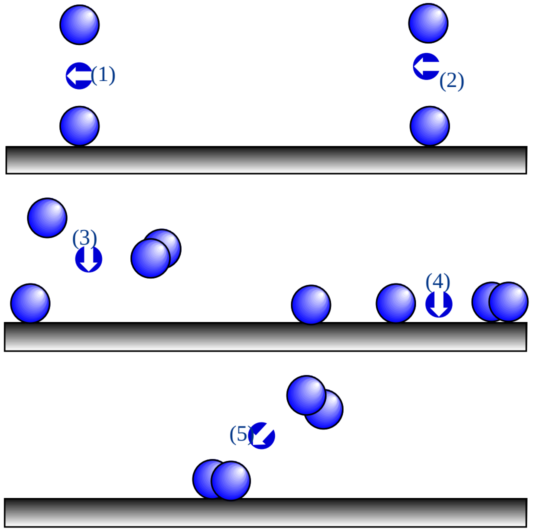
B. Bäuerle, F. Behrendt, F. Hoffmann

Stuttgart
- Hermes did Fly Nicely in Simulations

Temperature distribution for Hermes test case: Mach 25, height: 74 km, angle of attack: 30 deg



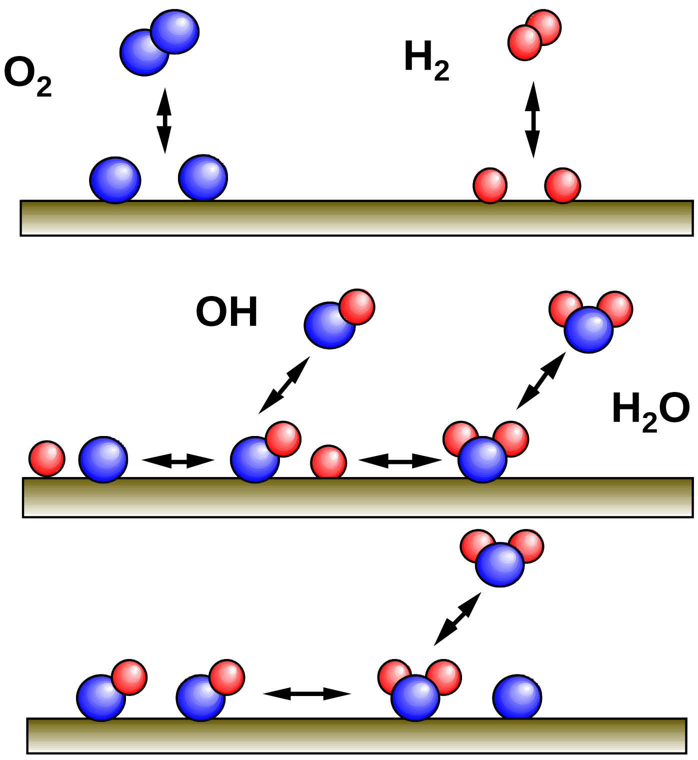
Surface Mechanism

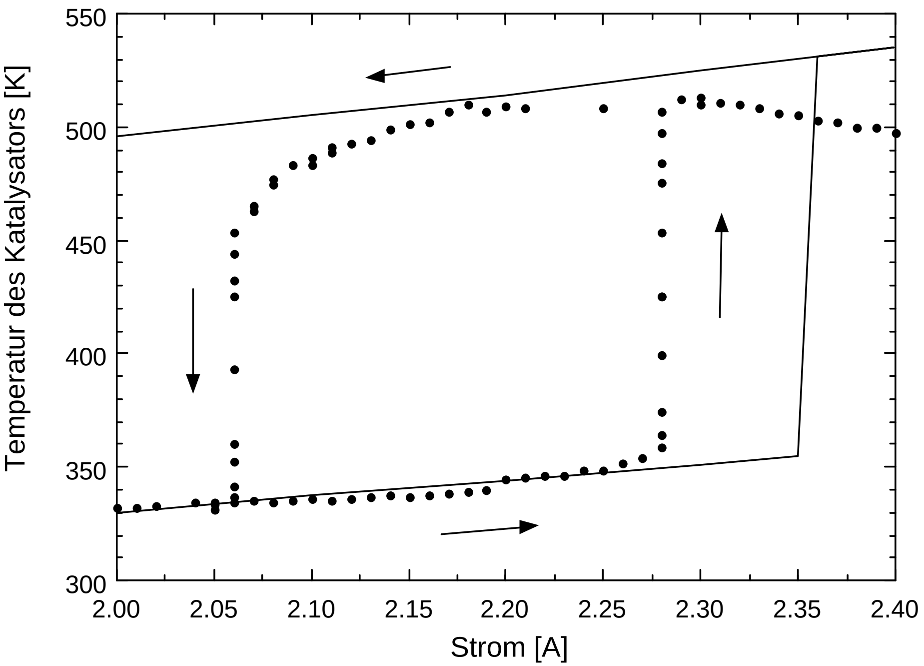


U. Maas, U. Riedel

Stuttgart
- Heterogeneous Reactions

First calculations of heterogeneous ignition processes





in cooperation with R. J. Kee et al., SNL/CRF

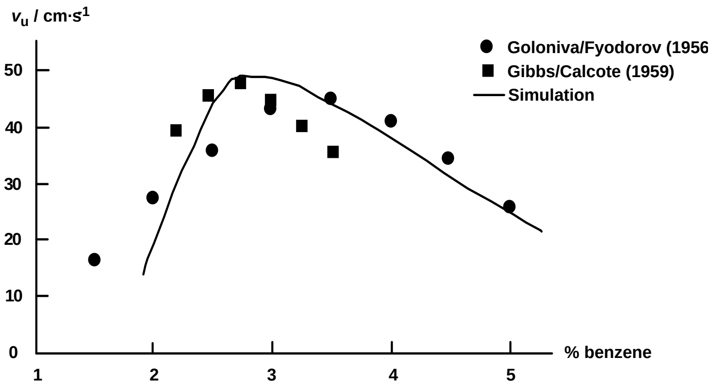
Being back in a More Diverse Heidelberg

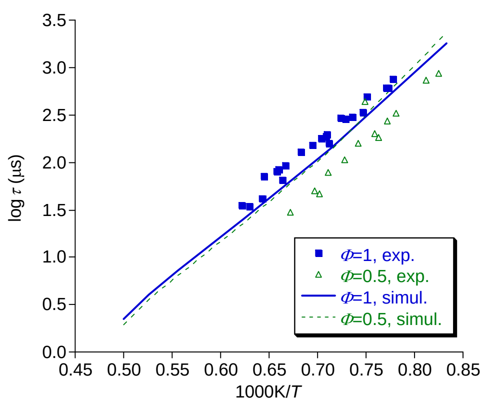
- Detailed and Reduced Chemistry
- Heterogeneous Ignition and Combustion
- Direct Numerical Simulation
- Engines
- Gas Turbines
- Solid-Oxide Fuel Cells

Heidelberg
- Detailed Chemistry

Flame velocities of benzene-air flames

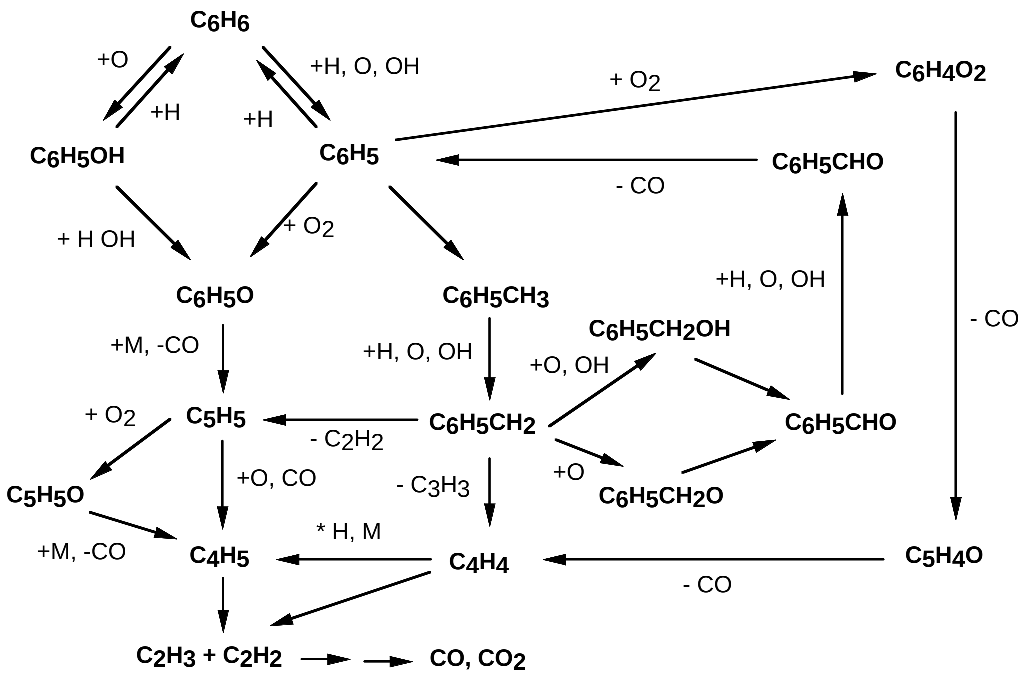
T_u = 298 K, p = 1 bar





Ignition delay times of benzene - O_2 - Ar

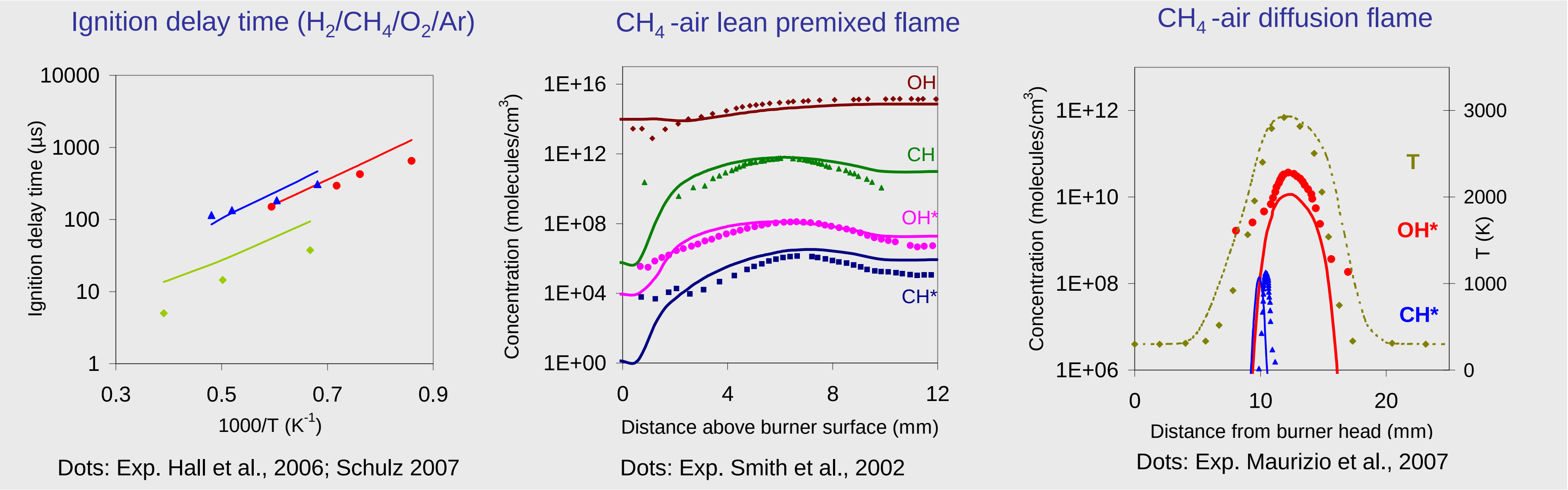
Φ = 0.5 and 1, p = 2 - 3 bar, exp: Burcat (1986)



V. Karbach

Heidelberg
- Detailed Chemistry Including Excited Species

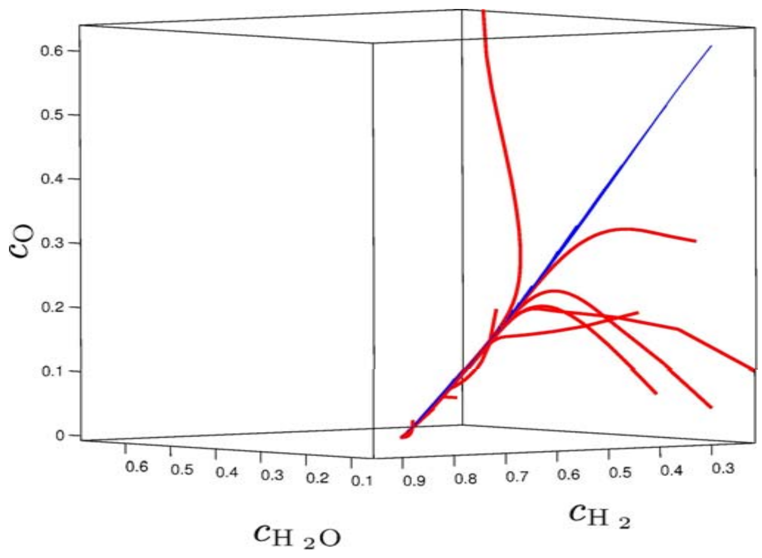
- **Development of reliable chemiluminescence - mechanism involving electronically excited OH*, CH*, C_2* and CO_2* species**
- **Analysis of available literature rate data**
- **Integration of CL - species/reactions into existing C_1 - C_4 oxidation mechanism**
- **Tools: Reaction flow analysis, sensitivity analysis**
- **Validation by simulation of shock tube experiments (0D) and laminar flames (1D)**

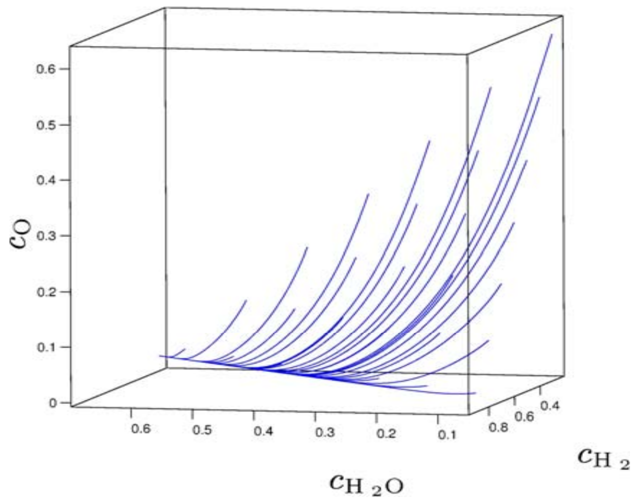


T. Kathrotia, U. Riedel

Heidelberg
- Reduced Chemistry

- **Trajectories in reaction systems relax to low-dimensional manifolds – slow invariant manifold (SIM)**
- **Modern model reduction approaches based on approximation of SIM (ILDM, CSP e.g.)**



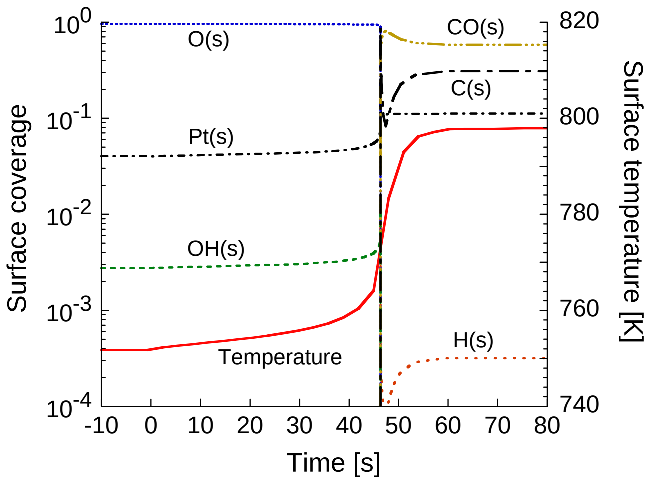


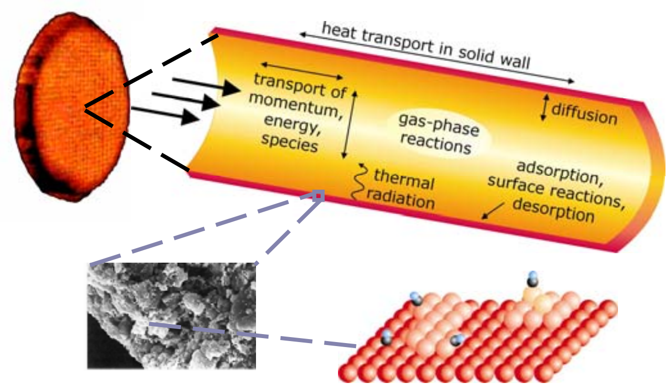
- **Boundary conditions (e.g. low temperatures) can impede solution of reduction equations**
- **Optimization approaches „guarantee“ solvability**
- **Sophisticated mathematical tools for optimization of trajectories**
- **Progress variables by fixing (some) initial concentrations**

H. Niemann, V. Reinhardt

Heidelberg
- Heterogeneous Ignition and Combustion

- **Catalytic combustion and ignition of H_2, CO and CH_4 on Pt and Pd**
- **Monte-Carlo model for CO oxidation on platinum**
- **Catalytic partial oxidation of higher aliphatic hydrocarbons**



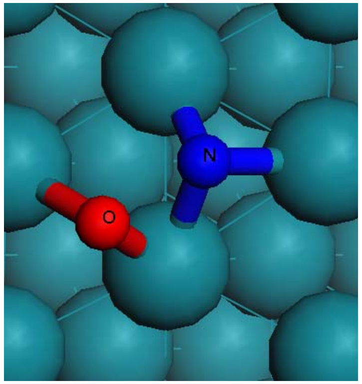


Zur Anzeige wird der QuickTime™ Dekompressor „TIFF (LZW)“ benötigt.

F. Behrendt
O. Deutschmann
R. Kissel-Osterrieder

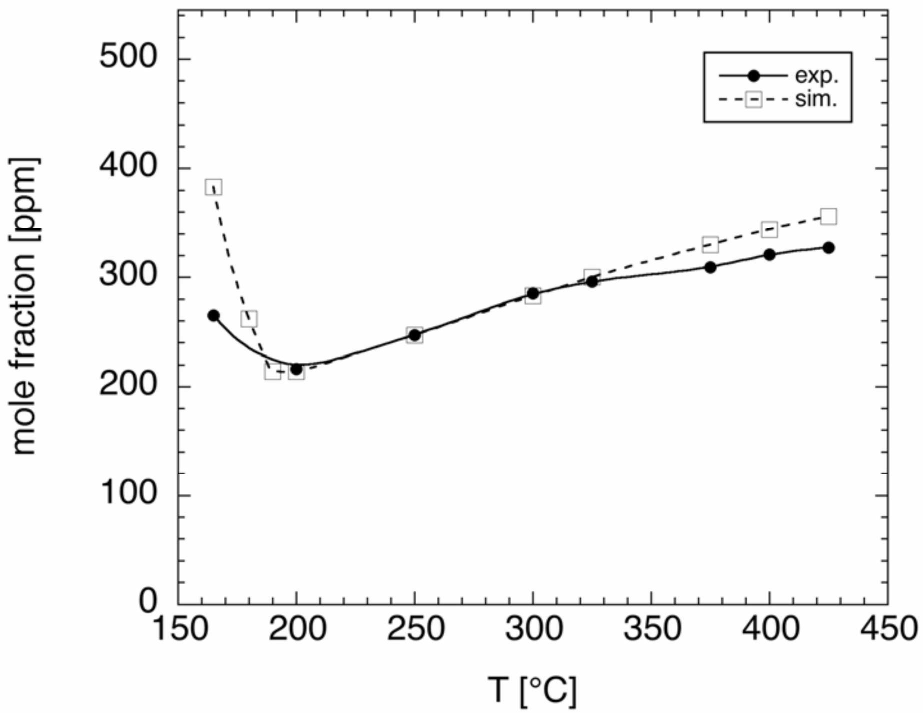
Heidelberg
- Automotive Exhaust Gas After-Treatment

Transition State of the
NO Dissociation on Rh{111}



DFT-aided mechanistic development

Averaged NO_x Emission over Lean-Rich Cycles



CONNECAT
KOMPETENZNETZWERKKATALYSE

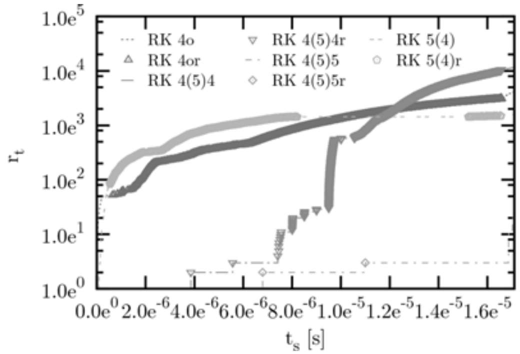
improved description of instationary emission control catalysts

O. Inderwildi

Heidelberg
- Direct Numerical Simulation

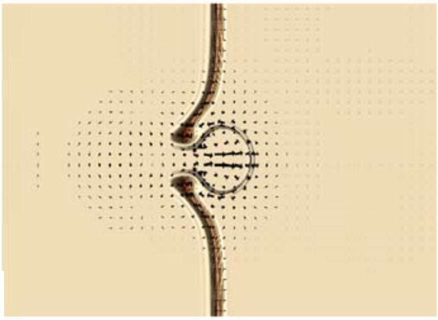
Time integration methods

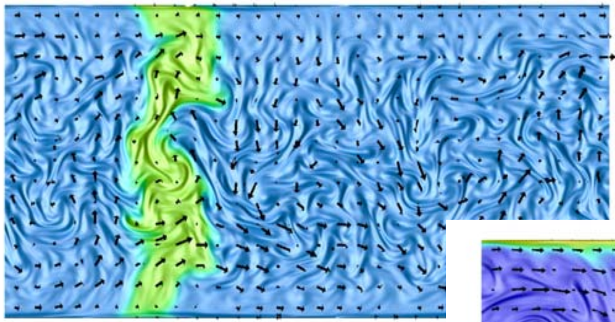
- Explicit higher order Runge-Kutta methods
- Richardson extrapolation and embedding
- Accuracy, efficiency, stability
- Non-reactive and reactive test cases



Flame-Vortex Interaction

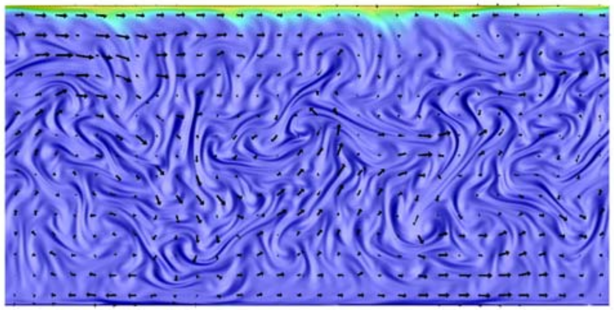
- Comparison of time integration scheme
- Methane mechanisms with 15/39 species
- Detailed models for chemistry and transport





Transport in turbulent channel flow

- Statistics, particle trace, spectra
- Re = 3500, 5000, 7000
- Transport of a initially flat NO-line

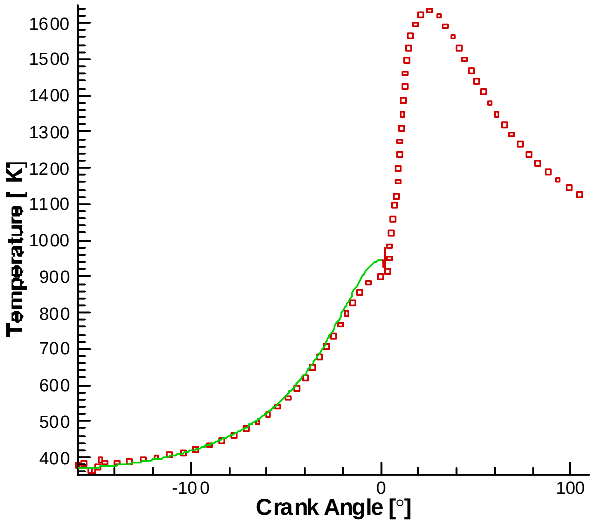


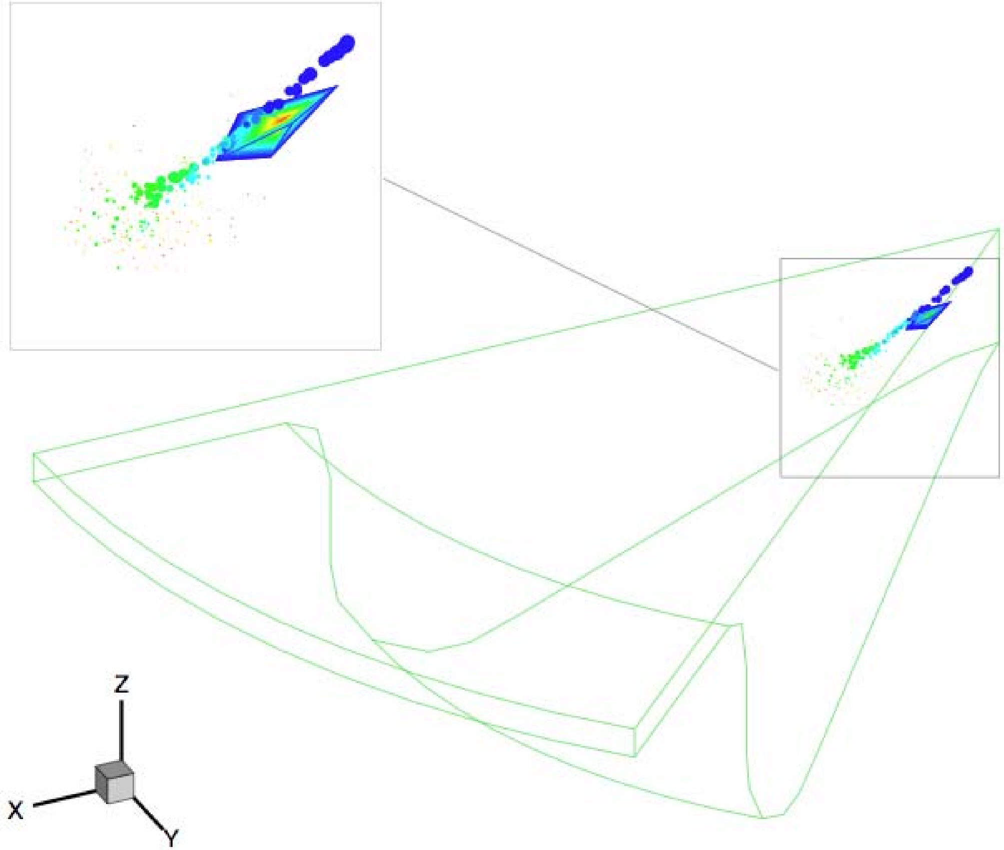
Investigation of the boundary layer

- Non-reactive: NO seeded boundary layer
- Reactive: catalytic wall

Heidelberg
- Engines

Description of Diesel Ignition and Combustion





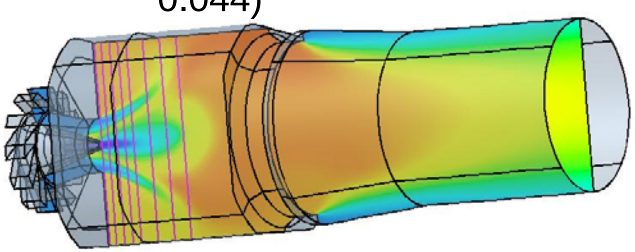
Correa, Gutheil, Elsden

Localizing the ignition point of the spray by the CO mole fraction

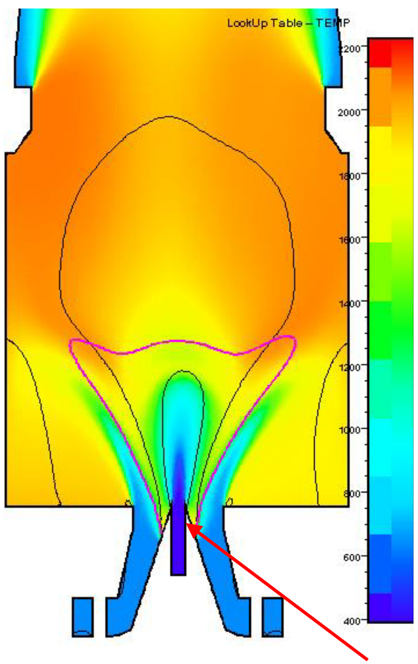
Heidelberg
- Advanced Gas-Turbine Combustion Chambers

Generic Combustor Rig (TU Darmstadt)

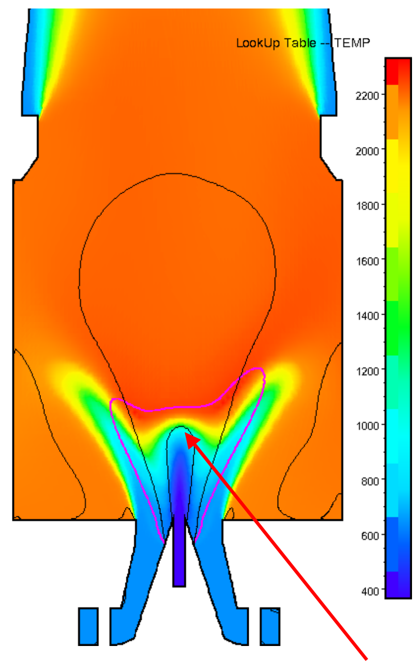
- Fuel: natural gas, T = 368 K
- Oxidiser: air, T = 623 K (m = 30 g/s)
- Characteristics of the flame
  - Coherent structures
  - Lifted
- Operating conditions:
  - Combustor pressure: p = 2 bar
  - Swirl number: S_0 = 1.2
  - Equivalence ratio λ = 0.8 (ϕ = 0.044)



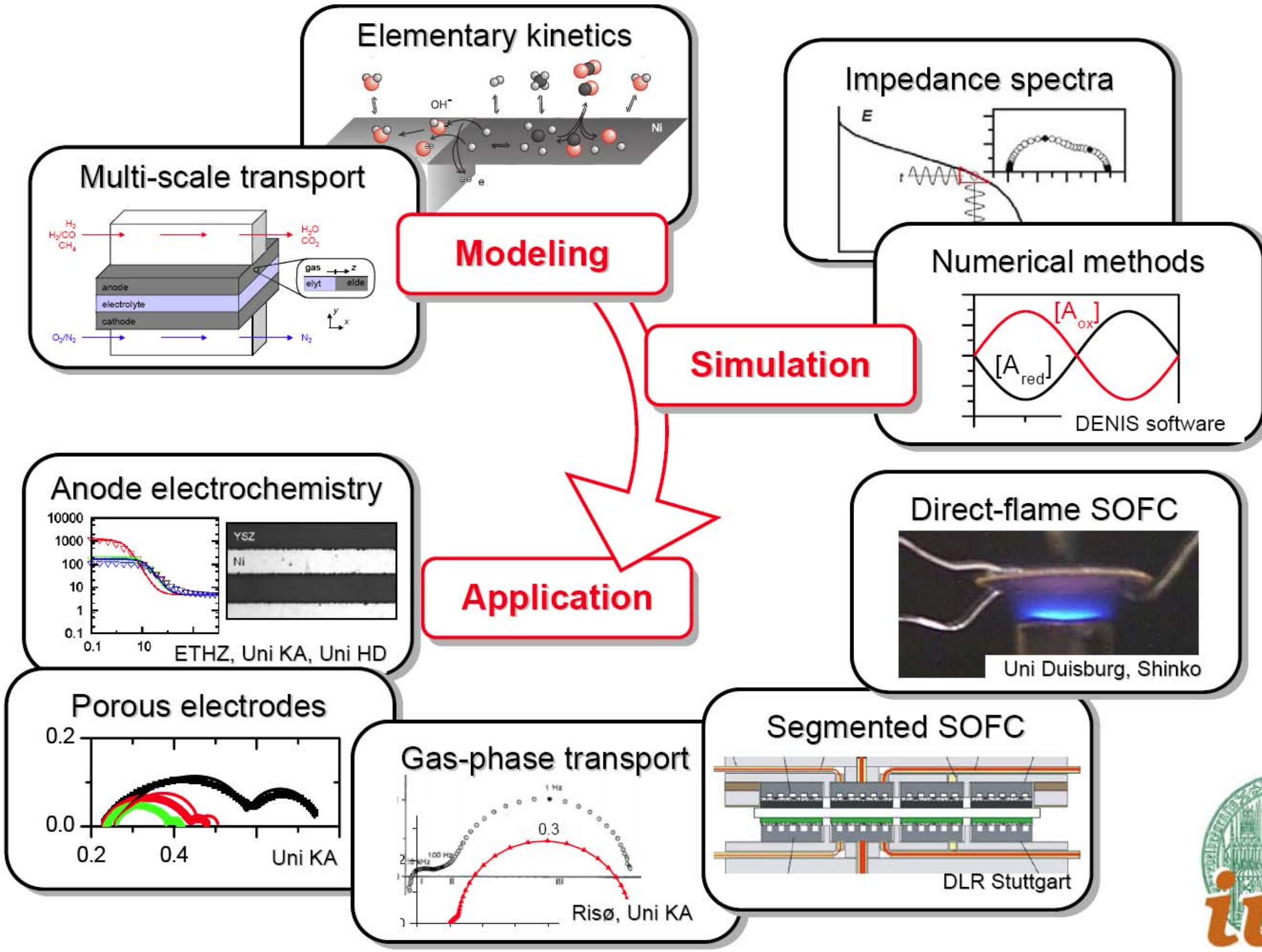
RANS / Flamelet



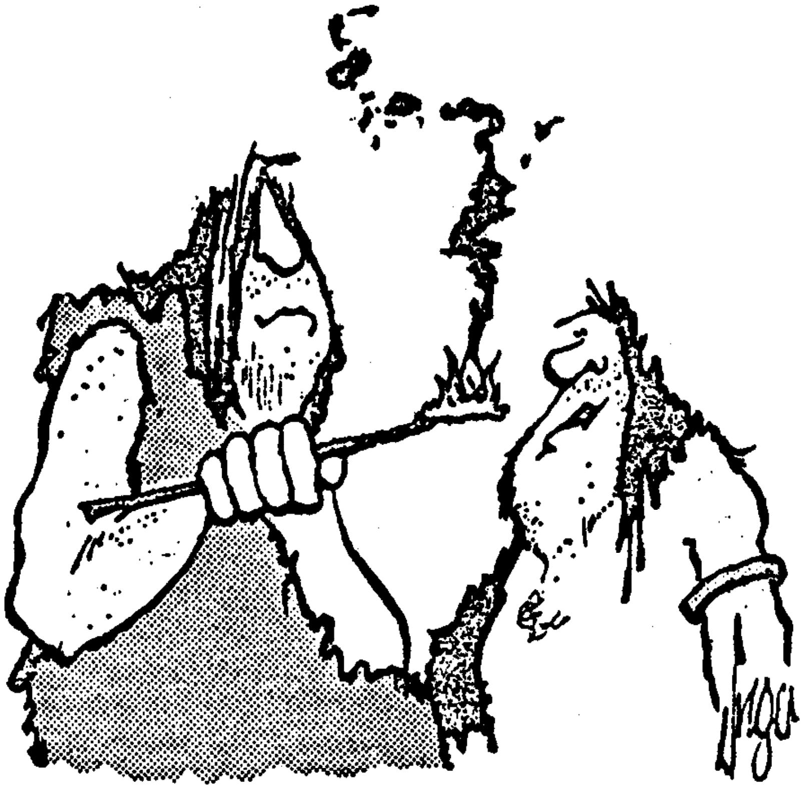
RANS / 1 progress variable (ILDM-based)



Heidelberg
- Solid-Oxide Fuel Cells



W. G. Bessler, S. Gewies, M. Vogler, V. Yurkiv, N. Bayer Botero, C. Hellwig, F. Backfisch



That's fantastic. I can't keep up with all
this modern technology