Reaction pathway visualization with FluxViewer++

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Reaction pathways

- Conversion of one species to another

„each arrow indicates a reaction step”

„the width of the arrows is proportional to the consumption rate of the reactant”

- This also means that the widths of the arrows in these figures cannot be compared to each other

⇒ **Flux of a conserved property has to be plotted!**

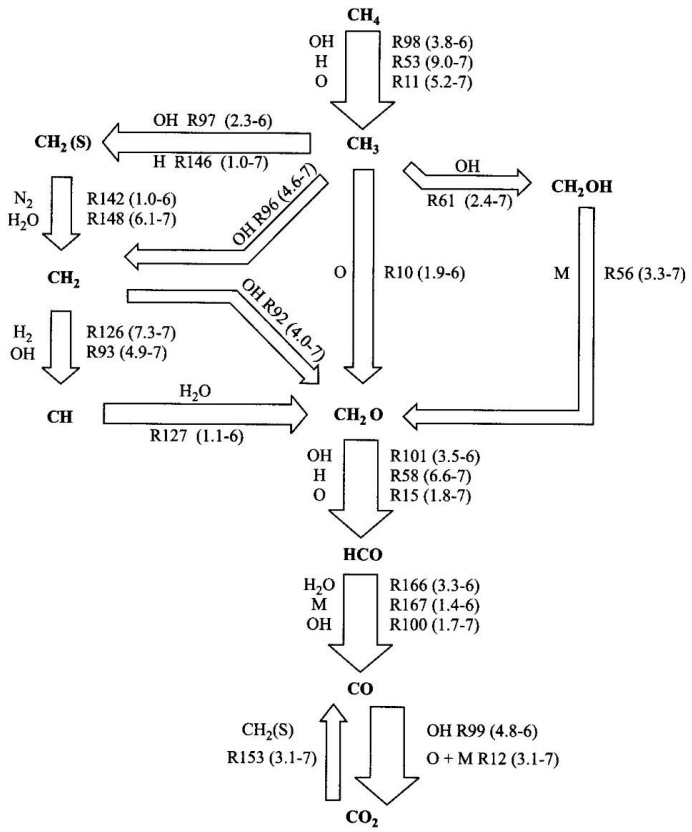


Figure 5.4 High-temperature reaction pathway diagram for combustion of methane in a well-stirred reactor at $T = 2200$ K and $P = 1$ atm for a 0.1-s residence time. Reaction numbers refer to Table 5.3, while reaction rates are shown in parentheses. For example, 2.6-7 implies $2.6 \cdot 10^{-7}$ (gmol/cm^3-s).

S.R. Turns: *An introduction to combustion. Concepts and applications*. second edition, Boston, McGraw-Hill, 2000.

Fluxes of elements

Flux of element A from species j to species k through reaction step i

$$A_{ijk} = \frac{n_{\mathrm{A},j}\, n_{\mathrm{A},k}\, r_i}{N_{\mathrm{A},i}}$$

- $n_{\mathrm{A},j}$ the number of atoms A in species j
- $n_{\mathrm{A},k}$ the number of atoms A in species k
- $N_{\mathrm{A},i}$ the sum of atoms A on either side of the reaction
- r_i the rate of reaction step i

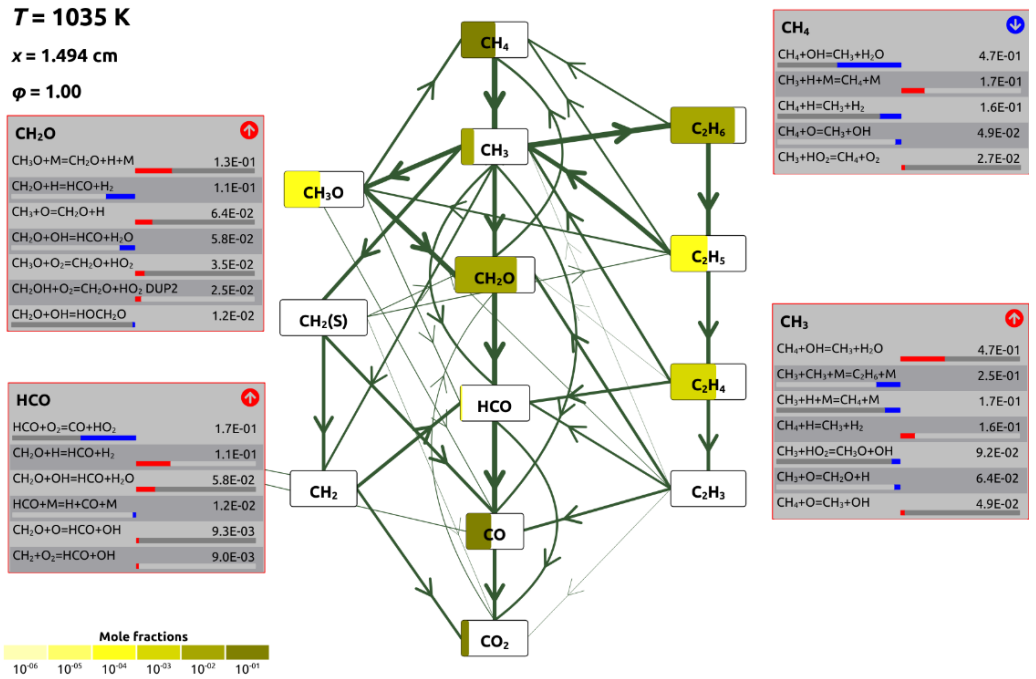
Sum of the element fluxes at a given reaction time t

$$A_{jk}(t) = \sum_i A_{ijk}(t)$$

J. Revel, J. C. Boettner, M. Cathonnet, J. S. Bachman, *J. Chim. Phys.* **91**, 365-382 (1994)

FluxViewer++

- Species as boxes
- Width of the arrow proportional to the log of the element fluxes
- Concentrations are color coded
- Animated visualization of how connections evolve with reaction progress



CH4 – air premixed flame
(T_0 = 300 K, p = 1 atm, φ = 1)

Optima++ – ATOMFLOW job

- Generates input files for FluxViewer++

```
ATOMFLOW
  MECHANISM Han-2023          ! Use the Han-2023 mechanism

  SOLVER        cantera       ! Use Cantera as solver

  ELEMENTS           N H O    ! Calculate the flux of
                              ! elements H, N and O

  POINTS_NUM         500      ! Print 500 points

  ! Use the following xml files
  NAME XMLs/x10100017.xml POINTS 1 OUTPUTS idt_Han2023
END
```

```
(ct-env) PS C:\Users\matyi\OptimaPP_respecth> .\bin\Release\OptimaPP.exe .\INPUTS\AtomFlow_NH3_H2_Han2023
```

Task – NH_3/H_2 ignition

- NH_3/H_2 ST-IDT experiment from B. Liu et al. (WUT), *Fuel* 371 (2024), 131850.
  - x10100017.xml first point (T = 1425 K, p = 10 atm, φ = 1.0, 95% Ar)
- Compare the reaction pathways using the following two mechanisms

ID	Reference
Han-2023	X. Han et al., *Appl. Energ. Combust. Sci*. 15 (2023) 100160.
NUIG-2024	Y. Zhu et al., *Combust. Flame* 260 (2024) 113239.