



SP2 Public Summary Report

*Based on the Del. 2.3.4:
Analysis and Reduction of the Final Reaction Mechanism*

*N.B. For a broader view on hydrogen combustion in gas turbines, this report should
be read together with the summary report of Del.2.3.3*

Authors:
Jochen Ströhle, Tore Myhrvold (SINTEF Energy Research)

This report should be cited as:
Ströhle and Myhrvold. Public summary report of ENCAP deliverable D2.3.4 Analysis and Reduction
of the Final Reaction Mechanism [online]. Available from Internet: www.encapco2.org

This study is part of work package WP 2.3 'H₂-rich combustion' of the European research project ENCAP. The main idea of this project is to convert fossil fuels to gas mixtures consisting mainly of hydrogen and carbon dioxide, and to separate CO₂ from the fuel prior to combustion in a gas turbine process. This necessitates the development of a gas turbine combustor for H₂-rich fuels.

The aim of this study is to find a reduced reaction mechanism that both efficiently and accurately represents H₂/O₂ kinetics over a large range of conditions, particularly for fuel lean mixtures at elevated pressures as present in a gas turbine combustor. Based on a thorough analysis of the detailed H₂/air mechanism of Li *et al.* (2004), several reduced mechanisms have been derived from the full detailed mechanism and tested for the prediction of laminar flame speed, ignition delay, and extinction using a 1D laminar flame code and a PSR model, respectively. Furthermore, these mechanisms have been applied to numerical simulations of two turbulent jet flames with the CFD code SPIDER using the EDC (Eddy Dissipation Concept) combustion model.

Table 1: Hydrogen mechanism of Li et al. (2004) in the form $k = A T^n \exp(-E/RT)$ for N₂ as the main bath gas. Units are cm, moles, s, cal, K.

No.	Reaction	A	n	E
1	H + O ₂ = O + OH	3.547×10^{15}	-0.406	16599
2	O + H ₂ = H + OH	0.508×10^{05}	2.67	6290
3	H ₂ + OH = H ₂ O + H	0.216×10^{09}	1.51	3430
4	O + H ₂ O = OH + OH	2.970×10^{06}	2.02	13400
5	H ₂ + M = H + H + M ^a	4.577×10^{19}	-1.40	104380
6	O + O + M = O ₂ + M ^a	6.165×10^{15}	-0.50	0
7	O + H + M = OH + M ^a	4.714×10^{18}	-1.00	0
8	H + OH + M = H ₂ O + M ^a	3.800×10^{22}	-2.00	0
9	H + O ₂ + M = HO ₂ + M ^b	$k_{\infty} 1.475 \times 10^{12}$ $k_0 6.366 \times 10^{20}$	0.60 -1.72	0 524.8
10	HO ₂ + H = H ₂ + O ₂	1.660×10^{13}	0.0	823
11	HO ₂ + H = OH + OH	7.079×10^{13}	0.0	295
12	HO ₂ + O = O ₂ + OH	0.325×10^{14}	0.0	0
13	HO ₂ + OH = H ₂ O + O ₂	2.890×10^{13}	0.0	-497
14	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂	4.200×10^{14}	0.0	11982
	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂	1.300×10^{11}	0.0	-1629.3
15	H ₂ O ₂ + M = OH + OH + M ^c	$k_{\infty} 2.951 \times 10^{14}$ $k_0 1.202 \times 10^{17}$	0.0 0.0	48430 45500
16	H ₂ O ₂ + H = H ₂ O + OH	0.241×10^{14}	0.0	3970
17	H ₂ O ₂ + H = HO ₂ + H ₂	0.482×10^{14}	0.0	7950
18	H ₂ O ₂ + O = OH + HO ₂	9.550×10^{06}	2.0	3970
19	H ₂ O ₂ + OH = HO ₂ + H ₂ O	1.000×10^{12}	0.0	0
	H ₂ O ₂ + OH = HO ₂ + H ₂ O	5.800×10^{14}	0.0	9557

^a third body enhancement factors: H₂=2.5, H₂O=12

^b third body enhancement factors: H₂=2, H₂O=11, O₂=0.78; Troe parameter: 0.8

^c third body enhancement factors: H₂=2.5, H₂O=11; Troe parameter: 0.5

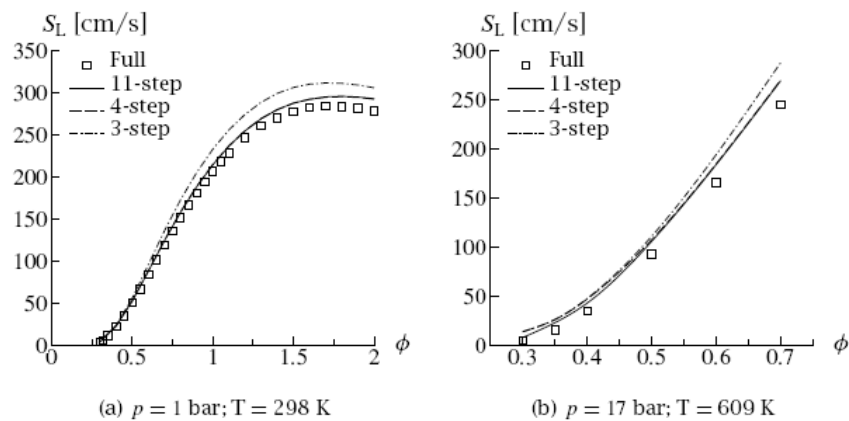


Figure 1: Example results: Laminar flame speed, S_L , for H_2 /air mixtures as function of equivalence ratio ϕ , computed with the full and reduced mechanisms.

The results show that at least 11 of the 19 elementary reactions are necessary for a satisfactory prediction of the processes of ignition, extinction, and laminar flame propagation under gas turbine conditions. A 4-step reduced mechanism using steady-state approximations for HO_2 and H_2O_2 yields excellent results for laminar flame speed and extinction limits, but fails to predict ignition delay, particularly at low temperatures (i. e. $T < 1200K$ at 17 bar). A further reduction to three steps using a steady-state approximation for O leads to significant errors for all these processes.

For the simulations of the two turbulent jet flames, both the 11-step skeletal and the 4-step reduced mechanism yield good agreement with the results of the full mechanism. The computational time of the 11-step skeletal mechanism decreases by 10% compared with the full mechanism. The 4-step mechanism leads to an increase in computational time, which can be explained by an increased stiffness of the mechanism. No converged solution could be achieved with the reduced 3-step mechanism.

The results of this study indicate that a reduction of the detailed mechanism has a large effect on the prediction of the isolated processes of laminar flame propagation, extinction, and particularly of auto-ignition, whereas the effect of the reduction becomes small for predictions of the investigated turbulent jet flames. However, the reduced mechanisms do not yield a significant reduction of computational effort. The 11-step skeletal mechanism constitutes the best choice concerning accuracy and computational time.

More information can be found in a published version of this study (Combustion and Flame, 144, 2006, 545-557).