

Übungen 1 zur Modellierung und Simulation IV (SS 2013)
[http://www.uni-ulm.de/mawi/mawi-numerik/lehre/sommersemester-2013/
 vorlesung-modellierung-und-simulation-4.html](http://www.uni-ulm.de/mawi/mawi-numerik/lehre/sommersemester-2013/vorlesung-modellierung-und-simulation-4.html)

Aufgabe 1.1 (Chemical Reaction Kinetics)

$$\sum_{s=1}^{n_{spec}} \nu'_{sr} X_s \rightleftharpoons \sum_{s=1}^{n_{spec}} \nu''_{sr} X_s, \quad r = 1, \dots, n_{reac}$$

$$q_r = k_{f,r} \prod_{s=1}^{n_{spec}} c_s^{\nu'_{sr}} - k_{r,r} \prod_{s=1}^{n_{spec}} c_s^{\nu''_{sr}}$$

$$\dot{c}_s = \sum_{r=1}^{n_{reac}} \nu_{sr} q_r$$

$$\nu_{sr} = \nu''_{sr} - \nu'_{sr}$$

Reaction		k_f	k_r
H ₂	\rightleftharpoons 2 H	2.0	216.0
O ₂	\rightleftharpoons 2 O	1.0	337.5
H ₂ O	\rightleftharpoons H + OH	1.0	1400.0
H ₂ + O	\rightleftharpoons H + OH	1000.0	10800.0
O ₂ + H	\rightleftharpoons O + OH	1000.0	33750.0
H ₂ + O	\rightleftharpoons H ₂ O	100.0	0.7714
