KEB-45251
Numerical Techniques for Process Modeling
Exercise 3 - Nonlinear systems
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Antti Mikkonen
Niko Niemelä

Problem 1

This problem is very similar to the course home assignment. We have hot air $T_{in} = 900\,\mathrm{K}$ entering a heat exchanger with free stream velocity $U_\infty = 5\,\mathrm{m/s}$. The pipes shown in Fig. 1 have a diameter $D = 6.35\,\mathrm{cm}$ and the pipe surface temperature is $T_s = 600\,\mathrm{K}$. The distance between pipe centers is $S_T = 2.5D$. We have $N_L = 100$ pipe in the flow direction and $N_T = 24$ pipes in parallel flow direction.

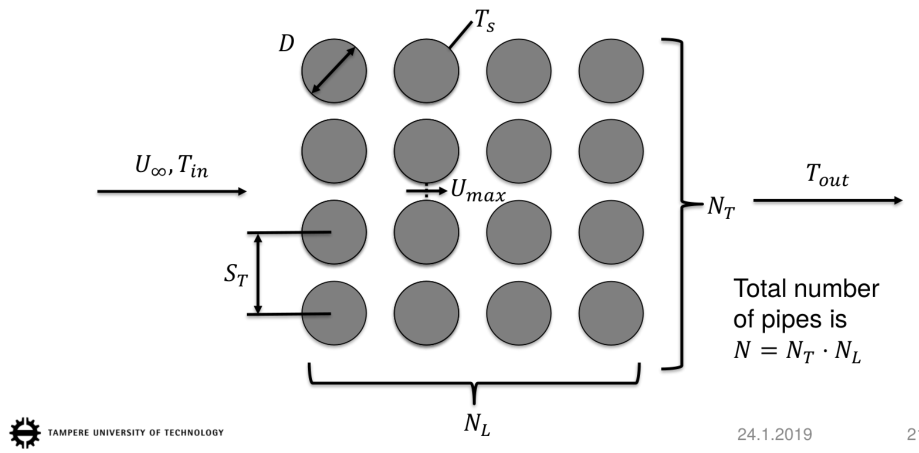

Figure 1: Heat exchanger, lecture slides.

Solve the outlet temperature T_{out} using

(a) **a for loop and under-relaxation.**

(b) **Scipy**.

See Scipy documentation for details.

Problem 2

Under stoichiometric methane combustion

When methane burns under stoichiometrically ($\lambda = a < 1$), there is insufficient amount of oxygen and the flue gas will contain multiple gas species, as shown in the following equation:

$$CH_4 + 2a(O_2 + 3.76N_2) \rightarrow bCO_2 + cCO + dH_2O + eH_2 + 2a \cdot 3.76N_2$$

The amounts of gases CO_2, CO, H_2O and H_2 in the combustion products can be solved using chemical equilibrium assumption. The governing equation set is:

C atom balance:	$b + c - 1 = 0$	Eq. 1
O atom balance:	$2b + c + d - 4a = 0$	Eq. 2
H atom balance	$d + e - 2 = 0$	Eq. 3
Water-Gas Shift equilibrium reaction:	$dc \cdot K_p(T) - be = 0$	Eq. 4

where the equilibrium constant K_p depends on temperature and is defined as:

$$K_p(T) = e^{0.31688+4.1778z+0.63508z^2-0.29353z^3}, \qquad z = \frac{1000}{T} - 1$$

The equation set contains three linear algebraic equations and one nonlinear algebraic equation. It can be solved for example using **fsolve** for known air-fuel ratio a and temperature T.

a) Solve the equilibrium composition of the combustion products for $a = \lambda = 0.8$, when the combustion products are in temperature $T = 1600\ K$.
b) Make a graph which shows the equilibrium composition for $0.3 \leq a \leq 1$, when the combustion products are in temperature $T = 1600\ K$.

Use the following notation in your Python code:

$$n = \begin{bmatrix} n_{CO_2} \\ n_{CO} \\ n_{H_2O} \\ n_{H2} \\ n_{N_2} \end{bmatrix} = \begin{bmatrix} b \\ c \\ d \\ e \\ 2a \cdot 3.76 \end{bmatrix} \quad \text{(mol)}$$

Result validation: From Eq. (1) in the following page, we can calculate the flue gas composition with $\lambda = 1$:

$$n_{tot} = n_{CO_2} + n_{H_2O} + n_{N_2} = 1 + 2 + 2 \cdot 3.76 = 10.52\ mol$$
$$x_{CO_2} = \frac{n_{CO_2}}{n_{tot}} = \frac{1\ mol}{10.52\ mol} = 9.51 \text{ mol-\%} = 9.5 \text{ vol-\%}$$
$$x_{H_2O} = \frac{n_{H_2O}}{n_{tot}} = \frac{2\ mol}{10.52\ mol} = 19.0 \text{ vol-\%}$$
$$x_{N_2} = \frac{n_{N_2}}{n_{tot}} = \frac{2 \cdot 3.76\ mol}{10.52\ mol} = 71.5 \text{ vol-\%}$$

In part b), check that your flue gas composition approaches this composition when $\lambda \rightarrow 1$.