Cantera: a simulation of pressure loss in a leaking tank

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1 Problem description

The goal of the project was to simulate the loss of pressure in a tank containing a mixture of flammable gases.

1.1 Simulation model

In the simulation the tank is treated as a zero - dimensional, thermically isolated reactor, from which the gases escape to the enviroment - a reservoir containing air. The leak is simulated by a valve.
The fuel consists of hydrogen, methane, ethane and propane in mole proportion set by user and is mixed with air or oxygen according to chosen equivalence ratio. The temperature and pressure of the mixture are also set by user.
Ignition in tank may or may not happen, depending on the beginning conditions. After the parameters are set, the program prints the state of gas at the beginning of the simulation..

1.2 Model of leakage

The leakage is simulated as a valve. Cantera uses model in which the mass of gas flowing through a valve is described by the following equation:
Q = KvΔ P
To determine the value of Kv another equation was used:
Q = $\alpha A\sqrt{(2g\rho}$ Δ P) [1]
Following these equations, Kv depends on two variables and the equation for Kv may be shown in the following way:

[1] Bomelburg, H.J.,1977,"Estimation of gas leak rates through very small orifices and channels."

$Kv = k\sqrt{(\rho/\Delta P)}$

Where the k factor depends on the size of the orifice and other factors that should be determined empyrically. In this simulations it is set constant:

$k = 0.001$

For calculations factor ρ is read as the density of gas inside the tank and ΔP is the difference in pressure inside and outside of the tank.

1.3 Solution

The simulation proceeds with time steps equal 0,01 s, for each step printing and saving to file the number of step, time, temperature and pressure. The name of the output file is "tankleak.csv".
At the end of the printed results of calculations the program generates two plots for pressure and temperature change in time.

1.4 Libraries

The simulation requires os, csv, cantera, matplotlib.pyplot and numpy libraries.

2 Sources

For modelling the leakage I have used equations provided in Bomelburg, H.J.,1977,"Estimation of gas leak rates through very small orifices and channels." As for programming solutions I have based on the Python examples provided on the Cantera homepage: "combustor.py" and "reactor2.py".