SD Toolbox: a simulation of detonation in a cylindrical tank

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June 11, 2019

1 Problem description

The goal of the project was to simulate the states of gas in a cylindrical tank after passing of a detonation and reflected shocks, using Cantera and SD Toolbox libraries in Python environment. Calculations were also meant to check if weld between cylinder and its lid is strong enough.

2 Simulation model

The initial state of gas contained in the tank, including mole fractions of fuel, equivalence ratio, oxidizer, pressure and temperature, is set by user.
The initial shock is implied to be Chapman - Jouguet detonation. Using the SDToolbox library, the program calculates the speed of shock wave. Basing on it and the initial state the program calculates the frozen state of gas after passing of the shock wave.
As the tank is closed, the most extreme conditions may appear in a frozen state after the reflected shock. Basing on the previously found values, this state is also calculated.
After calculations of these states, gas parameters are printed in order in which they were calculated.

3 Calculation of the tank lid weld strength

The tank is closed with a butt-welded on, flat lid. The weld is implied to be the weakest and most probable to fail part of the tank. External radius of the tank (r), thickness of the wall (b) and width of the weld (h) are set by user.
To check if the tank will withstand the shocks, the program compares the allowable strength for the weld and the effective strength caused by high pressure inside the tank. The effective force is treated

as constant and the allowable force does not consider high temperatures in the tank.

For calculation of the effective force, the program chooses the higher of pressures in frozen after-shock state.

$p_{ef} = p_s - p_{atm}$

$A_p = \pi * (r - b)^2$

$F_{ef} = p_{ef} * A_p$

The area of weld is a disc with external radius equal r and width equal h.

$A_w = (\pi$ * $\mathrm{r}^2) - A_p$

Allowable tensile strength for weld equals 91.5 MPa.[1] Safety factor for calculation of allowable strength for weld is set to 1.5.

$F_{all} = \sigma_{all} * A_w/1.5$

4 Output

After calculations, the program prints values of following variables:

- area of weld
- area of shock
- allowable force
- force after shock

If the force after shock exceeds allowable value, the program prints "The weld is too weak". Otherwise, the output text is "The weld is strong enough."

5 Libraries

The simulation requires os, csv, cantera, sdtoolbox and numpy libraries.

6 Sources

For programming solutions I have used Python examples provided on the SD Toolbox homepage: "demo reflected fr", http://shepherd.caltech.edu/EDL/PublicResources/sdt/doc/QuickReferenceSDT.pdf, 11.06.2019.

I have used the allowable weld tensile strength value provided in: IIT Kharagpur, "Design of welded joints, Version 2 ME", https://nptel.ac.in/courses/112105125/pdf/mod10les4.pdf, 11.06.2019

[1] IIT Kharagpur,"Design of welded joints, Version 2 ME", https://nptel.ac.in/courses/112105125/pdf/mod10les4.pdf, 11.06.2019