Development of Key-Enabling Technologies for a Variable-blend Natural Gas Vehicle

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A Research Report from the National Center for Sustainable Transportation

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U.S. Department of Transportation (USDOT) Disclaimer

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EXECUTIVE SUMMARY

A portable, economic and reliable sensor for the Natural Gas (NG) fuel quality has been developed. Both Wobbe Index (WI) and Methane Indexes (MI) as well as inert gas content (inert%) of the NG fuel can be measured in real time within 5% accuracy. This sensor is targeting to be used in any equipment that involves NG combustion including NG vehicle, boiler, building HVAC, various consumer level gas appliance and Variable Natural Gas Vehicle (VNGV). The VNGV is an NG vehicle that can operate on any arbitrary mixture of CH_4 and CO_2, thus allowing the use of Renewable Natural Gas (RNG) including biogas for transportation without comprehensive gas cleanup/upgrading.

The technology behind is to predict the "Value of Interests" (WI, MI and inert%) by the signals from easily "Measurable Physical Properties" (such as thermal conductivity, temperature, etc..), as shown in the figure.

Prediction of "Value of Interest" by data mining (esp. Multivariate Analysis and/or Artificial Neural Network) is the key idea of the concept. This technology is non-invasive, rugged, and small in size promising to overcome limitations and shortcomings such as bulky size and intrusive nature of conventional measurement technology.

VNGV technology will enable widespread use of RNG as a transportation fuel, resulting in significant reductions in GHG emissions in the transportation sector.

Introduction

Renewable Natural Gas (RNG), i.e., natural gas produced from renewable feedstocks (e.g., Landfill gas, biomass, etc.) is an important alternative fuel that can contribute to achieving a number of goals set by the local and federal governments related to fossil fuel replacement and greenhouse gas (GHG) emissions reduction in the transportation sector. Natural Gas Vehicles (NGVs) have achieved reasonable market penetration over the past decade. However, a significant increase in the number of NGVs running on RNG is needed in order to make an impact on net GHG and criteria pollutant emissions reduction. Most RNG production projects are small to medium scale by nature and comprehensive gas cleanup/upgrading to meet NGV fuel specifications is often not feasible from a project economic perspective. This results in most RNG resources being wasted (e.g., flaring) or being left unused. Developing NGVs that can accept a broader range of RNG fuel properties is critical to achieve widespread RNG usage in transportation.

We aim to develop key technologies that are necessary to advance the Variable Natural Gas Vehicle (VNGV) concept to commercialization. The VNGV would run on conventional natural gas, but could also operate on any arbitrary mixture of natural gas and RNG contained in its on board compressed gas storage tank. The Figure below shows conceptual diagram of VNGV (ECU = Engine Control Unit).

The two technologies needed by a VNGV are: (1) on-board detection of fuel properties and (2) adaptive combustion control for a wide range of fuel variations.

On-board detection of fuel properties is an essential part of adaptive engine control determining the engine combustion mode and combustion control, and integration of emission control systems. Among the fuel properties, Wobbe Index (WI), the ratio of a calorific value of a fuel to the square root of its specific gravity, is a well-known, critical factor for fuel interchangeability. WI is not only related to VNGV, but is also used in a wide variety of equipment and processes that involve natural gas combustion. WI is typically measured using bulky, complex and expensive analyzers. These devices measure the energy value of the fuel by direct calorimetry followed by separate measurement of density by an optical method. The complex, destructive, and expensive nature of existing WI measurement systems prevent its use for automotive applications, especially as an on-board diagnostic sensor.

The new WI sensor which uses a combination of thermal conductivity with predictive measurement technology is developed. The conceptual diagram of the sensor is provided in Figure 1. This technology is non-invasive, rugged, and small in size and can overcome the limitations such as bulky size and intrusive nature of conventional WI measurement technology. The fuel sensor is not only measure WI, but also Methane Index (MI), which is a critical parameter for engine operation. Since MI provides an indication of the knocking tendency of the fuel, while WI provides the energy value of the fuel, both are regarded as critical parameters for the adaptive engine control of VNGV.

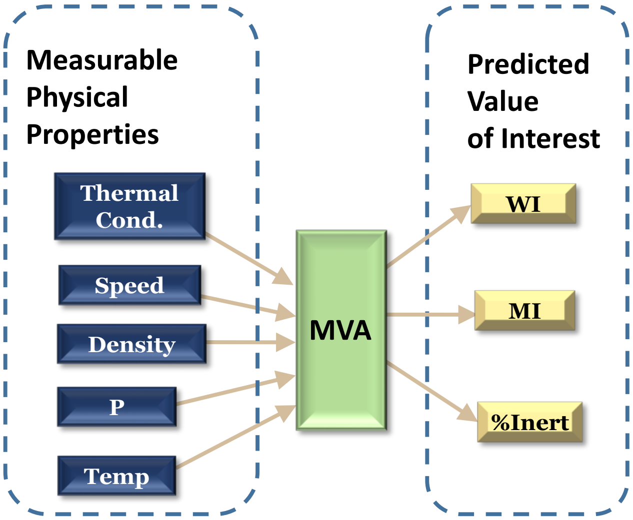

Figure 1. Conceptual Logic Diagram of the Sensor

The sensor also can estimate the inert gas content (i.e. Nitrogen, CO2) of fuel, which can be as high as ~50% in RNG sources. This is an important parameter as it guides the Exhaust Gas Recirculation (EGR) control strategy of the engine to minimize criteria pollutant emissions.

Scope of Work

The project consists of two tasks as described below.

Task 1: Database Development

A database of blended fuel compositions was completely constructed. Existing compositional information of biogas from landfill, anaerobic digesters and household waste together with those from fossil sources was used. Measurable Physical Properties of each blended fuel mixture at varying pressures and temperatures was calculated by CHEMKIN transport module, which includes thermal conductivity, mass/mole density and sound velocity.

Task 2: Develop WI and MI sensor Algorithm

Value of Interest (WI, MI) was also estimated using Aspen Plus simulation model from the known compositional information. Inert gas composition was directly collected from the composition, without relying on simulation. Using the MVA model in MATHLAB, relationships between “Measurable Physical Properties” and the “Values of Interest” was developed. Final result shows, prediction algorithm can successfully estimate the WI and inert% of the fuel within 2% and 1% each.

Result and Discussion

Task 1: Fuel Sensor Database Development

The variation of natural gas composition in the pipeline is dependent of the geographical region and the variation in composition can affect the thermodynamic properties of the gas mixture. In addition to the published composition of RNG, the list of pipeline gas mixture selected for this study is listed in Table 1.

Table 1. Composition of the Fuel Gas Blends

Gas	Methane (mol%)	Ethane (mol%)	Propane (mol%)	CO_2 (mol%)
Texas pipeline	96	1.8	0.4	0.95
Rocky Mountain pipeline	94.5	3.5	0.6	0.75
Peruvian LNG	88.3	10.5	0	0
Associated high ethane	83.65	10.75	2.7	0
Associated high propane	87.2	4.5	4.4	0

According to the proposed idea of gas mixture blending the 5 different (Texas pipeline, Rocky Mountain pipeline, Peruvian LNG, Associated high ethane, Associated high propane) gas mixture is taken. The blending composition varies by 10% for individual gas mixture. An example of the blending composition is shown in Table 2.

Table 2. Blending Composition Variation of the Gas Mixture

Blend	Texas pipeline (%)	Rocky Mountain pipeline (%)	Peruvian LNG (%)	Associated high ethane (%)	Associated high propane (%)
1	0	10	10	10	70
2	10	10	10	10	60
3	20	10	10	10	50
4	30	10	10	10	40

A wide range of temperature and pressure is used for the property calculation: -20° to 80° C with 20° C incremental interval, 500 psi to 3000 psi with 500 psi interval. Therefore, 6 different temperature and 6 different pressure can make 36 possible combination.

The detailed modelling concept requires calculation of several indirect variables as well as Wobbe Index and Methane Number at variable temperature, pressure and composition to establish the database. Specific indirect variables are: thermal conductivity (k), sound velocity (c). In order to calculate the sound velocity constant pressure heat capacity (Cp), constant volume heat capacity (Cv) are also necessary to calculate. All these parameters are calculated as a function of temperature, pressure and composition of the gas mixture.

Thermal Conductivity

Chemkin, a proprietary software tool for solving complex chemical kinetics problems, is used for calculating the thermal conductivity of the gas mixtures. The equations for calculating thermal conductivity of gas mixtures uses the thermal conductivity of individual components. To calculate the thermal conductivity we will use:

$$k_{\mathrm{M}} = \sum x_i k_i$$

where k_i is thermal conductivity of the ith component and x_i is the composition of ith component in the mixture. This equation will work since we will pull the real gas thermal conductivity values off the Chemkin software. k_i for each of the components are not done yet.

Sound Velocity

To calculate sound velocity we will use:

Sound velocity, c = , $\mathrm{c} = \sqrt{\frac{\gamma ZRT}{M}}$

$\gamma = \frac{C_p}{C_v}$

Z = compressibility factor (you already have this data from graph)

R = universal gas constant (8.314 J/(mol.K))

M = molecular weight of the gas mixture

In this, the gamma can be calculated by taking the ratio of specific heats at constant pressure and volume. These specific heats can be calculated using the following:

Specific Heat

To calculate specific heat we will use:

$$C_{P_M} = C_{P_A} y_A x_A + C_{P_B} y_B x_B + C_{P_C} y_C x_C + C_{P_D} y_D x_D$$

$$C_{V_M} = C_{P_M} - R$$

$$MW_{avg} = MW_A \cdot y_A \cdot x_A + MW_B \cdot y_B \cdot x_B + MW_C \cdot y_C \cdot x_C + MW_D \cdot y_D \cdot x_D$$

C_p and C_v for individual components at 36 different combinations of temperature and pressure are already done.

Wobbe Index

The Wobbe index calculation was performed by using Aspen Plus process simulator.

Methane Number

The Methane number property was taken from the following website where composition of the gas mixture is the only input. http://www.cumminswestport.com/fuel-quality-calculator

Figure 2 shows the sample database developed for the biogas mixed with natural gas and RNG from anaerobic digester gas.

	A	B	C	D	E	F	G	H	I	J
1	Constant			Thermal Conductivity	Sound Velocity	Wobbe Index	Methane number	Composition		
2		Temperature	Pressure	W/(m.K)	m/s	MJ/Nm3	MI (%)	CH4	C2H6	CO2
3		C	PSI					%	%	%
4	1	-20	500	0.027368	350.861031	54.90323934	84.5	94	6.00	0
5	1	-20	500	0.0270229	343.8976955	52.15534246	88.8	91.83	5.40	2.77
6	1	-20	500	0.0266779	336.4758299	49.53320114	93.2	89.66	4.80	5.54
7	1	-20	500	0.0263328	330.2904148	47.02575657	97.6	87.49	4.20	8.31
8	1	-20	500	0.0259877	324.4338765	44.62343969	102	85.32	3.60	11.08
9	1	-20	500	0.0256427	318.8777547	42.31766622	106.4	83.15	3.00	13.85
10	1	-20	500	0.0252976	313.5973835	40.10094715	110.7	80.98	2.40	16.62
11	1	-20	500	0.0249525	307.7832198	37.9664985	115	78.81	1.80	19.39
12	1	-20	500	0.0246074	303.0037533	35.90833625	119.2	76.64	1.20	22.16
13	1	-20	500	0.0242624	298.4399542	33.92108467	123.3	74.47	0.60	24.93
14	1	-20	500	0.0239173	294.0766435	31.99983964	127.3	72.3	0.00	27.7
15	1	-20	500	0.0237995	292.7374189	31.51045603	128.1	71.52	0.00	28.48
16	1	-20	500	0.0241446	297.0403301	33.41329195	124.2	73.69	0.60	25.71
17	1	-20	500	0.0236817	291.415903	31.02612868	129	70.74	0.00	29.26
18	1	-20	500	0.0244897	301.5389863	35.38081166	120.1	75.86	1.20	22.94
19	1	-20	500	0.0240268	295.6603121	32.91097738	125	72.91	0.60	26.49
20	1	-20	500	0.023564	290.1124122	30.5467886	129.8	69.96	0.00	30.04
21	1	-20	500	0.0248347	306.2485664	37.41768159	115.9	78.03	1.80	20.17
22	1	-20	500	0.0243719	300.0957228	34.85914559	121	75.08	1.20	23.72
23	1	-20	500	0.023909	294.2992678	32.4139818	125.9	72.13	0.60	27.27
24	1	-20	500	0.0234462	288.8263139	30.07229576	130.7	69.18	0.00	30.82

Figure 2. Sample Wobbe Index and Methane Number Database

Task 2: Find the Predictive Relationship for Wobbe Index and Methane Index

The sets of equation that can be used to predict Wobbe Index or Methane Index:

R = Xθ

X is represented as the matrix that includes all the variables. R is the matrix representing the wobble index or methane number.

For Wobbe Index:

$$\mathrm{X} = \left[1\ \frac{1}{T}\ \frac{1}{P}\ \frac{1}{k}\ \frac{1}{v}\right]$$

Where T = temperature; P = pressure; k = thermal conductivity; v = sound velocity

$$\theta = \begin{bmatrix} -7 \\ 55861 \\ 315 \\ -4 \\ -1204 \end{bmatrix}$$

The % of Root Mean Squared (RMS) error is: 3.75%

For Methane Number:

$$\mathrm{X} = \left[1\ \frac{1}{T}\ \frac{1}{P}\ \frac{1}{k}\ \frac{1}{v}\ \frac{1}{WI}\right]$$

Where T = temperature; P = pressure; k = thermal conductivity; v = sound velocity; WI = Wobbe Index

$$\theta = \begin{bmatrix} 186 \\ -4068.5 \\ -22.9 \\ 0.4 \\ 24.7 \\ -1.9 \end{bmatrix}$$

The % of RMS error is: 0.48%

For Inert Percentage:

$$\mathrm{X} = \left[1\ \frac{1}{\exp\left(-\frac{1}{T}\right)}\ \frac{1}{P}\ \frac{1}{k}\ \frac{1}{v}\ \frac{1}{WI}\right]$$

Where T = temperature; P = pressure; k = thermal conductivity; v = sound velocity; WI = Wobbe Index

$$\theta = \begin{bmatrix} 16 \\ -468.5 \\ -203.9 \\ 2.54 \\ 25.7 \\ 0.16 \end{bmatrix}$$

The % of RMS error is: 0.51%

Figures 3, 4, and 5 show the comparison of predicted versus actual Wobbe index, Methane Number and Inert percentage respectively. It shows the deviation from the perfect prediction, which would be a straight line with 45° angle with both vertical and horizontal axis. The deviation has been improved as the expansion of the sensor database by the learning mechanism of the prediction algorithm.

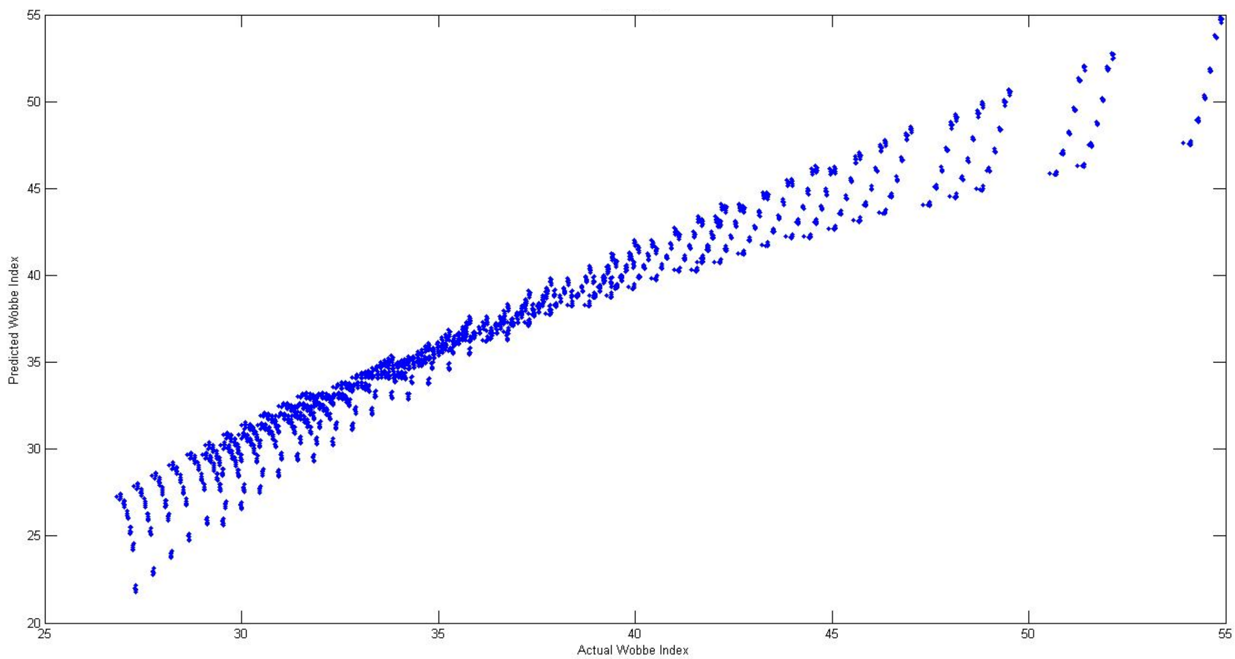

Figure 3. Predicted Wobbe Index by Using the Developed Model vs Actual Wobbe Index

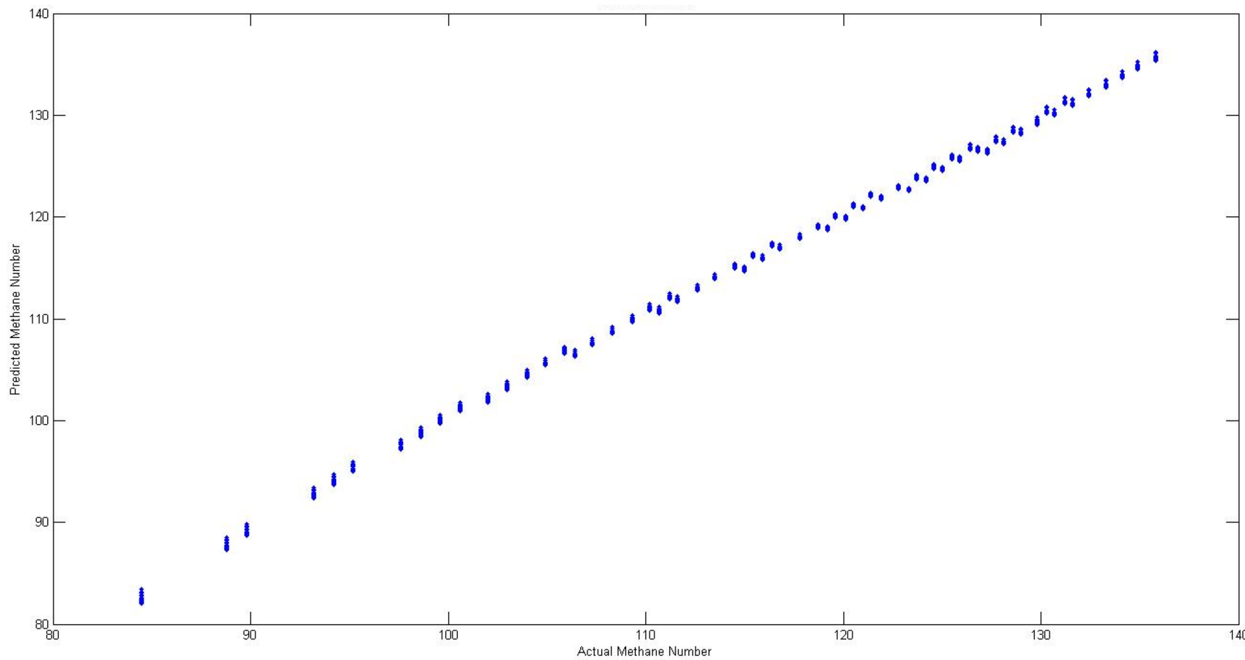

Figure 4. Predicted Methane Number by Using the Developed Model vs Actual Methane Number

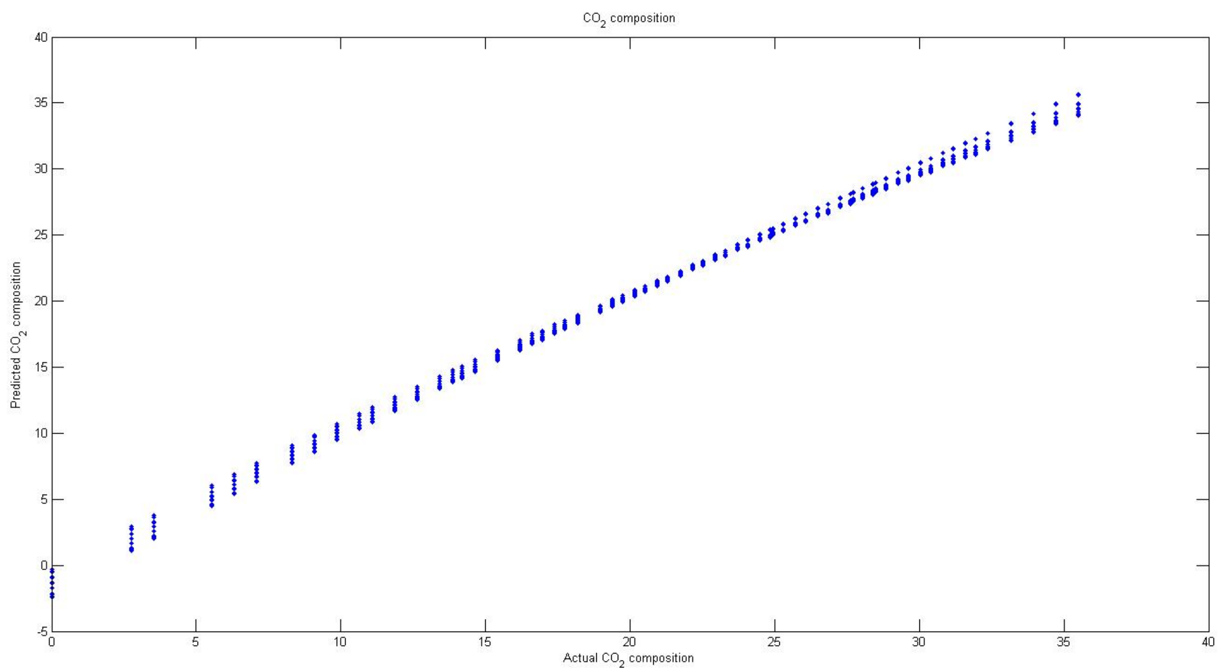

Figure 5. Predicted Inert Percentage by Using the Developed Model vs Actual Inert Percentage

Suggested Next Steps

The deviation in the prediction can be improved by learning mechanism of the prediction algorithm as further refined database is developing. Once the database for the composition and compressibility factor is improved thru further iteration, ɣ (by using Cp, Cv), k, and sound velocity as well as Wobbe index and methane number calculation will be refined for a better precision. The current database has been expanded containing around 40,000 combinations.

Sensor Prototype is currently developing although this is not scope of NCST work.

The engineering for the sensor prototype and Initial 3D modeling drawing for the sensor prototype is shown in Figure 6.

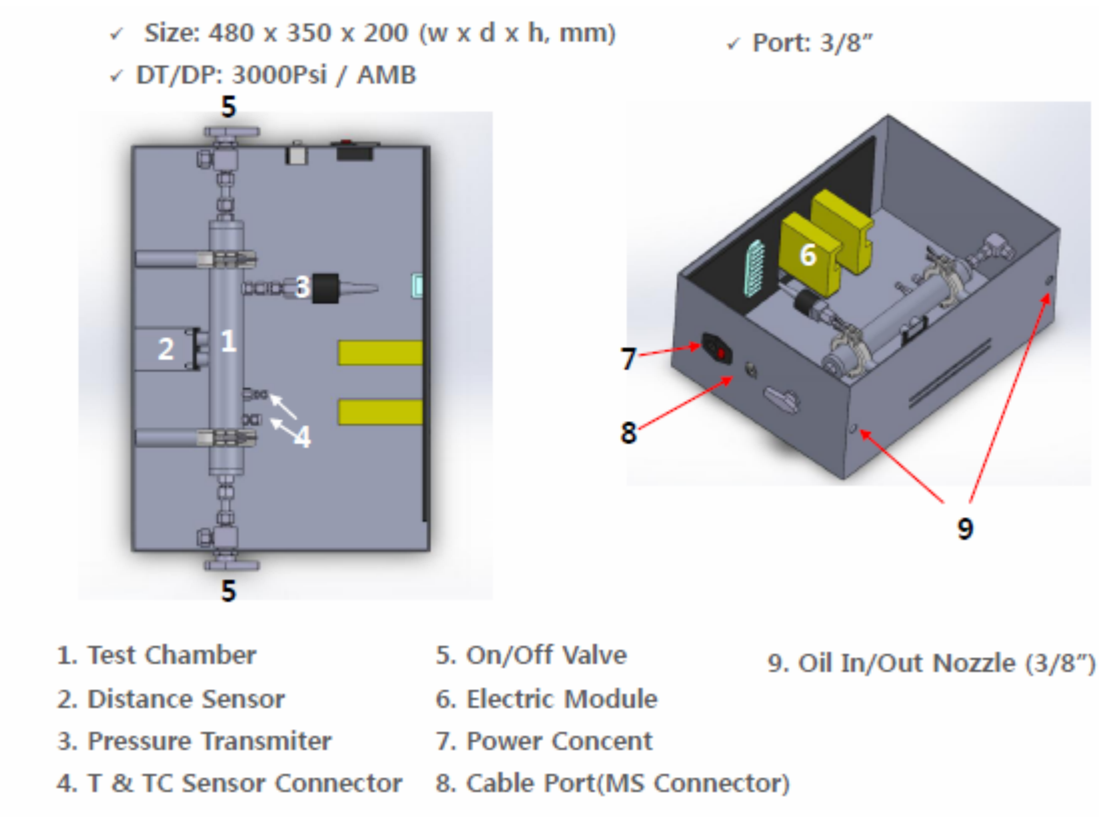

Figure 6. The Engineering Diagram for the Sensor Prototype and 3D Modeling

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