DEPARTMENT OF MECHANICAL ENGINEERING

Submitted for ME3112: Metrology and Instrumentation

Monte Carlo Simulation

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1 Problem Statement

The real efficiency of a fuel cell is given by

$$\eta_R = \frac{\Delta G * E_R}{\Delta H * E_I} \tag{1}$$

Compute the mean, standard uncertainty and 95% coverage interval for real efficiency of fuel cell using MCS using 2x105 trials. Plot histogram representing the resulting PDF for the real efficiency of a fuel cell estimated by Monte Carlo simulation.

Table 1: Measurand Details

Input Source	Type	PDF	PDF Parameters
Gibbs Free Energy ΔG	B	Uniform	Min: 236.0 kJ/mol;Max:236.4 kJ/mol
Enthalpy of formation ΔH	B	Uniform	Min: 283.6 kJ/mol; Max:284.8 kJ/mol
Ideal Voltage E_I	B	Triangular	Mean :1.3995 V, Min: 1.389 V ; Max:1.410 V
Real Voltage E_R	B	Uniform	Min: 0.6318 V ; Max:0.6825 V

2 Theory

Estimation of measurement uncertainties is a fundamental process for the quality of every measurement. In order to harmonize this process for every laboratory, ISO (International Organization for Standardization) and BIPM (Bureau International des Poids et Mesures) gathered efforts to create a guide on the expression of uncertainty in measurement. This guide was published as an ISO standard – ISO/IEC Guide 98-3 "Uncertainty of measure- ment - Part 3: Guide to the expression of uncertainty in measurement" (GUM) – and as a JCGM (Joint Committee for Guides in Metrology) guide (JCGM 100:2008). This document provides complete guidance and references on how to treat common situations on metrology and how to deal with uncertainties.

2.1 GUM Uncertainty Framework and Its Limitations

GUM uncertainty framework is the application of the law of propagation of uncertainty and the characterization of the output quantity by a Gaussian distribution or a scaled and shifted t distribution in order to provide a coverage interval.The GUM uncertainty framework is currently still the most extensive method used on estimation of measurement uncertainty in metrology. But law of propagation of uncertainties presented by the GUM is based on some assumptions, that are not always valid . The assumptions of GUM uncertainity framework are

- The model used for calculating the measurand must have insignificant non-linearity. When the model presents strong elements of non-linearity, the approximation made by truncation of the first term in the Taylor series used by the GUM approach may not be enough to correctly estimate the uncertainty output.

- Validity of the central limit theorem, which states that the convolution of a large number of distributions has a resulting normal distribution. Thus, it is assumed that the probability dis- tribution of the output is approximately normal and can be represented by a t-distribution. In some real cases, this resulting distribution may have an asymmetric behavior or does not tend to a normal distribution, invalidating the approach of the central limit theorem.

- After obtaining the standard uncertainty by using the law of propagation of uncertainties, the GUM approach uses the Welch-Satterthwaite formula to obtain the effective degrees of free- dom, necessary to calculate the expanded uncertainty. The analytical evaluation of the effec- tive degrees of freedom is still an unsolved problem, and therefore not always adequate.

In addition, the GUM approach may not be valid when one or more of the input sources are much larger than the others, or when the distributions of the input quantities are not sym- metric. The GUM methodology may also not be appropriate when the order of magnitude of the estimate of the output quantity and the associated standard uncertainty are approxi- mately the same.

2.2 Propagation of Distribution Approach

In order to overcome the limitations of propagation of uncertainty approach of GUM, methods relying on the propagation of distributions have been applied to metrology. This methodology carries more information than the simple propagation of uncertainties and generally provides results closer to reality. Propagation of distributions involves the convolution of the probability distributions of the input quantities, which can be accomplished in three ways:

1. Analytical integration
2. Numerical integration
3. Numerical simulation using Monte Carlo methods

The GUM Supplement 1 (or JCGM 101:2008) provides basic guidelines for using the Monte Carlo simulation for the propagation of distributions in metrology. It is presented as a fast and robust alternative method for cases where the GUM approach fails. This method provides reliable results for a wider range of measurement models as compared to the GUM approach.

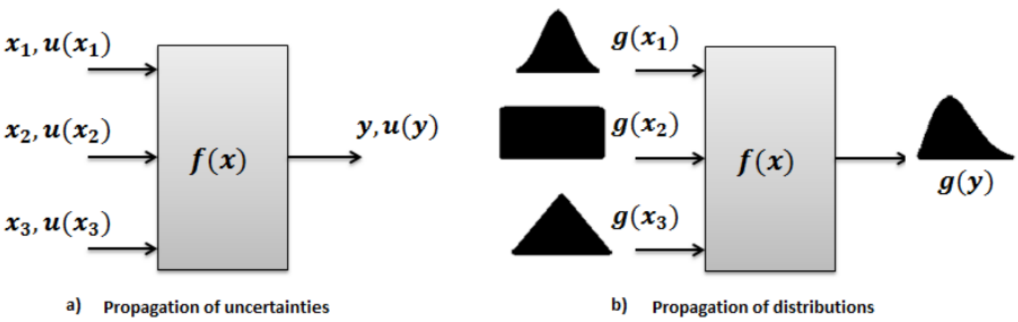

Figure 1: Comparison of Propagation of Uncertainty Approach and Propagation of Distributions approach

2.3 Monte Carlo Simulation(MCS)

The Monte Carlo methodology as presented by the GUM Supplement 1 involves the propagation of the distributions of the input sources of uncertainty by using the model to provide the distribution of the output. The sequence of steps to be followed for MCS as per GUM supplement 1 is

1. Definition of the measurand and input quantities
2. Modelling
3. Estimation of the probability density functions (PDFs) for the input quantities
4. Setup and run the Monte Carlo simulation
5. Summarizing and expression of the results.

3 Methodology

Monte Carlo Simulation (MCS) is implemented in Python by following the general steps of MCS. Number of trial ,M = 200000 (from problem statement).

3.1 Generating MCS Trials

M data points are drawn for each input quantity from the respective PDFs.PDF types and parameters are obtained from Table 1 .

1. Gibbs Free Energy ΔG
   M samples are drawn from uniform distribution with a minimum value of 236.0 kJ/mol and a maximum value of 236.4 kJ/mol. Mean of sampled data is 236.20000144084676 kJ/mol and standard uncertainty is 0.11564302861064871 kJ/mol, which are very close to the true values of mean (236.2 kJ/mol) and standard uncertainty ($\frac{0.2}{\sqrt{3}}$ kJ/mol)

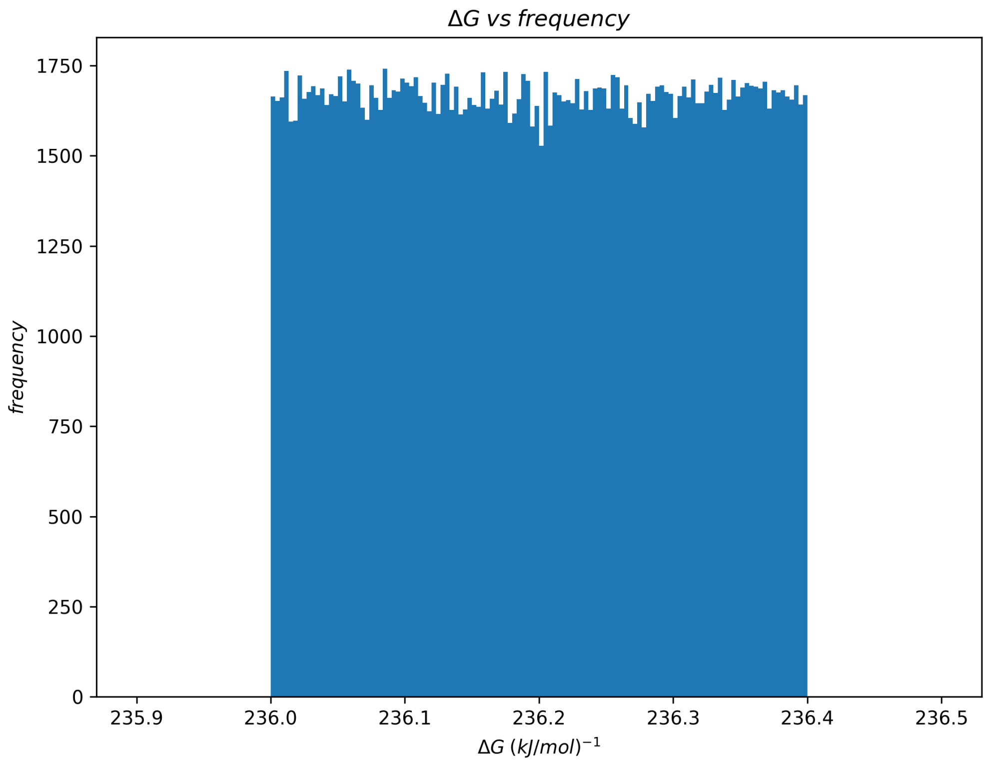

Figure 2: Histogram representing Samples of ΔG

2. Enthalpy of Formation ΔH
   M samples are drawn from uniform distribution with a minimum value of 283.6 kJ/mol and a maximum value of 284.8 kJ/mol. Mean of sampled data is 284.20014363974406 kJ/mol and standard uncertainty is 0.34650214189689693

kJ/mol, which are very close to the true values of mean (284.2 kJ/mol) and standard uncertainty ($\frac{0.6}{\sqrt{3}}$ kJ/mol)

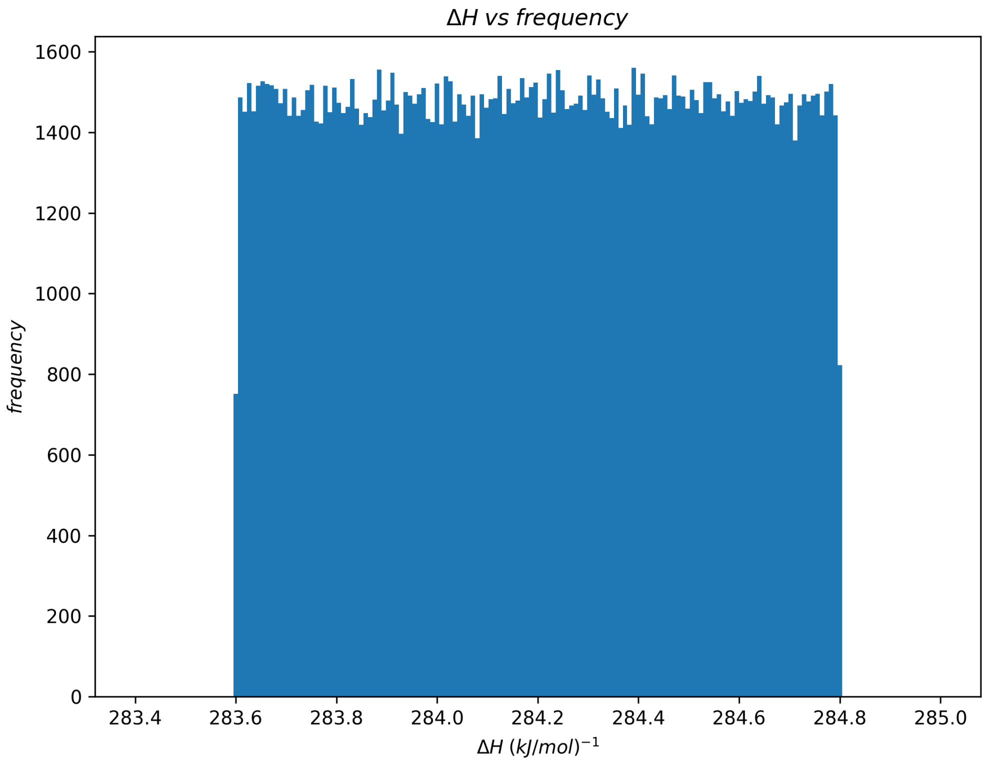

Figure 3: Histogram representing Samples of ΔH

3. Ideal Voltage E_I
   M samples are drawn from triangular distribution with a minimum value of 1.389 V ,maximum value of 1.410 V and mean of 1.3995 V. Mean of sampled data is 1.3995140357712266 V and standard uncertainty is 0.0042835503699681626 V. Once again sample mean and standard deviation are very close to the true values of mean (1.389 V) and standard uncertainty (0.00428660705 V)

4. Real Voltage E_R
   M samples are drawn from uniform distribution with a minimum value of 0.6318 V and a maximum value of 0.6825 V. Mean of sampled data is 0.6570847223480427 V and standard uncertainty is 0.01461622309658553 V kJ/mol, which are very close to the true values of mean (0.65715 V) and standard uncertainty ($\frac{0.02535}{\sqrt{3}}$ V)

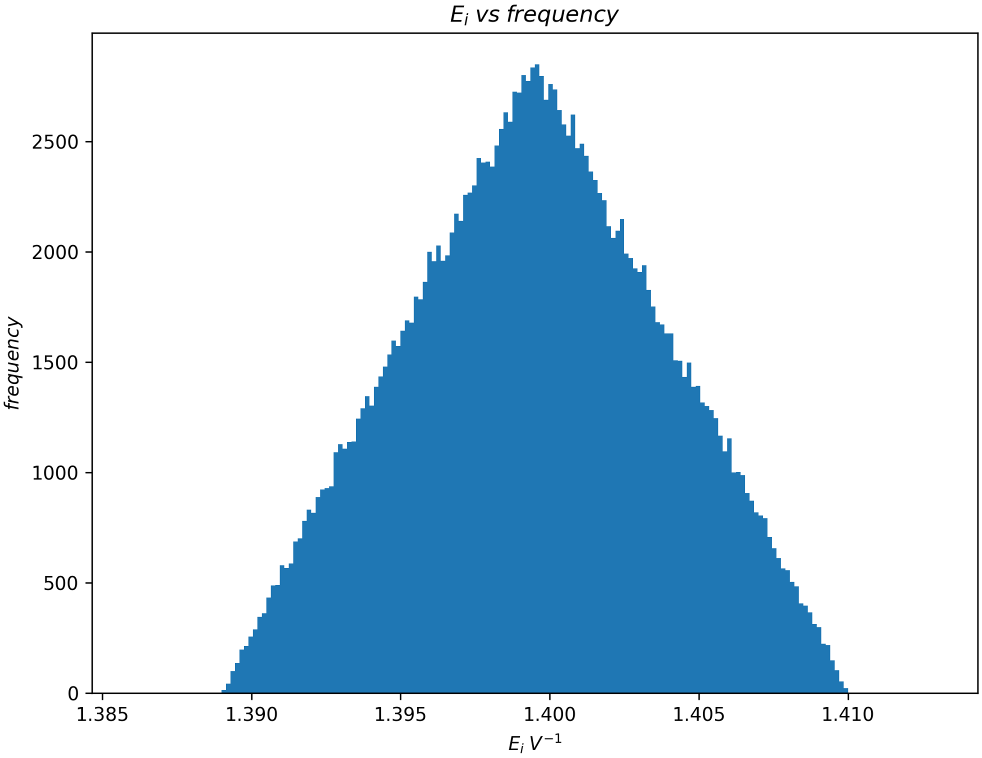

Figure 4: Histogram representing Samples of E_I

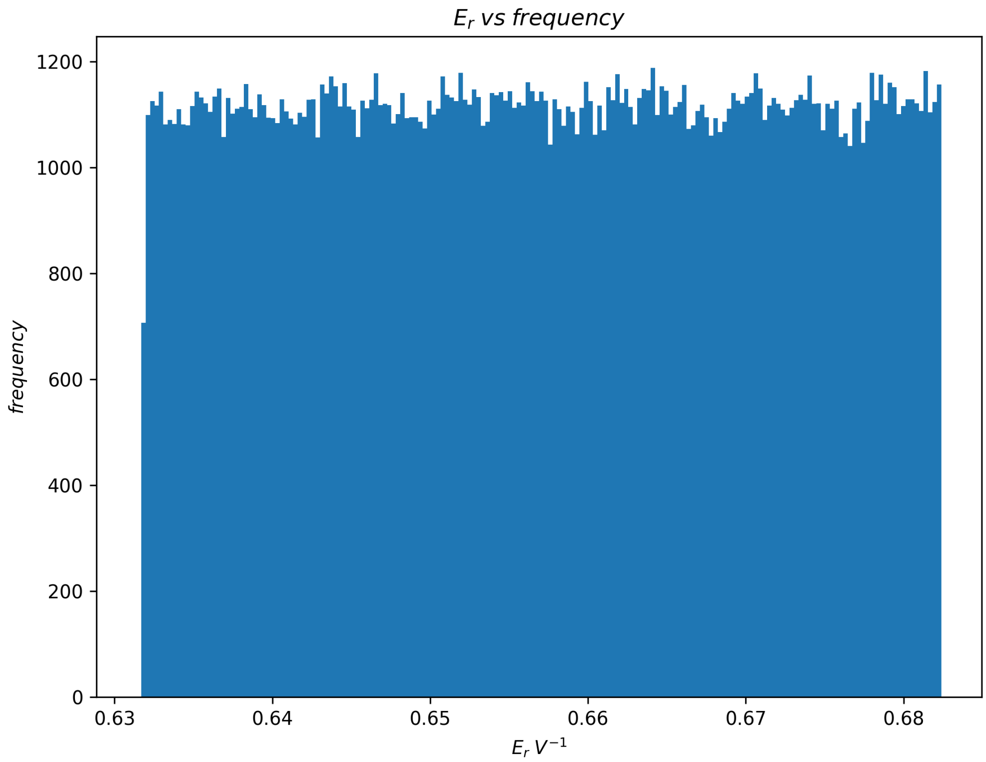

Figure 5: Histogram representing Samples of E_R

3.2 Model Evaluation and Sorting

Each of the M trials obtained in the previous step is plugged into the model equation 1 to evaluate the generate the samples. This data is then sorted to find out coverage interval.

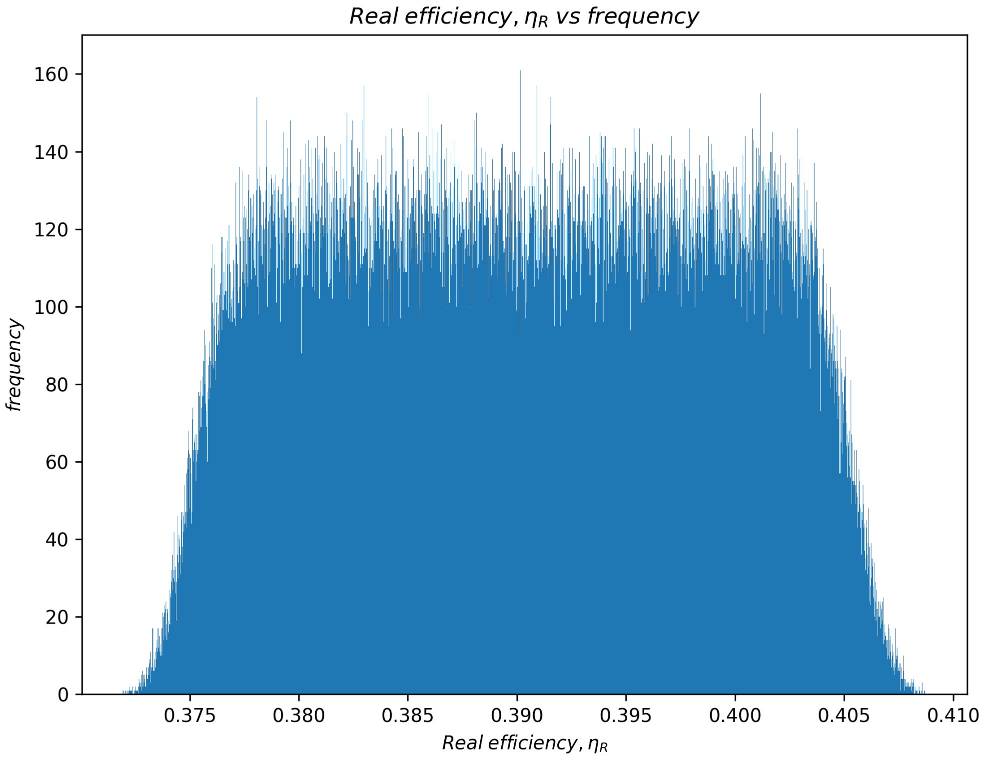

Figure 6: Histogram representing the resulting PDF for the real efficiency of a fuel cell estimated by Monte Carlo simulation

3.3 Determination of Coverage Interval

The coverage interval for 95% confidence is determined by truncating the resultant sorted data to remove 2.5% data from each side. Mean of the evaluated data is 0.3902197737987234 . The coverage interval for 95% confidence is (0.37562842658651535, 0.40492047063903513) .

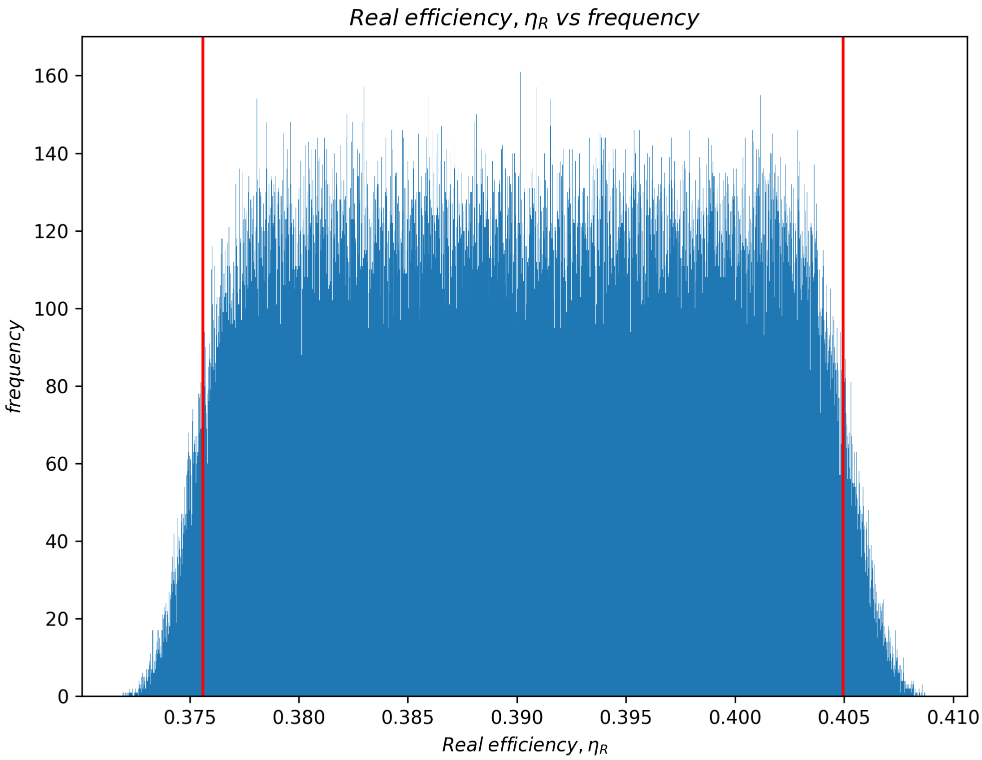

Figure 7: 95% Coverage Interval for η_R

4 Program

```
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams["figure.figsize"] = (8.5,6.5)

"""$$\eta_R = \dfrac{G  E_R}{H  E_I},$$ where:
$$ _R : \text{Real Efficiency of fuel cell} \\
G : \text{Gibbs Free Energy} \\
H : \text{Enthalpy of Formation} \\
E_I : \text{Ideal Voltage} \\
E_R : \text{Real Voltage}$$
"""

N = 200000 #sampling size

PDF_dG = np.random.uniform(236.0,236.4,N) #Uniform distribution for Delta G
plt.hist(PDF_dG,bins = np.linspace(235.9,236.5,181))
plt.title(r"$\Delta G\; vs\; frequency$")
plt.xlabel(r'$\Delta G\;{(kJ/mol)}^{-1}$')
plt.ylabel(r'$frequency$')
plt.show()
print(f"Delta G is a uniform distribution with mean:{PDF_dG.mean()} kJ/mol \\
    and standard uncertainity:{PDF_dG.std()} kJ/mol")

PDF_dH = np.random.uniform(283.6,284.8,N) #Uniform distribution for Delta H
plt.hist(PDF_dH,bins = np.linspace(283.4,285.0,181))
plt.title(r"$\Delta H\; vs\; frequency$")
plt.xlabel(r'$\Delta H\;{(kJ/mol)}^{-1}$')
plt.ylabel(r'$frequency$')
plt.show()
print(f"Delta H is a uniform distribution with mean:{PDF_dH.mean()} kJ/mol \\
    and standard uncertainity:{PDF_dH.std()} kJ/mol")

PDF_Ei = np.random.triangular(1.389,1.3995,1.410,N) #Triangular distribution \\
for E_i
plt.hist(PDF_Ei,bins = np.linspace(1.386,1.413,181))
plt.title(r"$E_i\; vs\; frequency$")
plt.xlabel(r'$E_i\; {V}^{-1}$')
plt.ylabel(r'$frequency$')
plt.show()
print(f"Ei is a triangular distribution with mean:{PDF_Ei.mean()} V and \\
    standard uncertainity:{PDF_Ei.std()} V")

PDF_Er = np.random.uniform(0.6318,0.6825,N) #Uniform distribution for E_r
plt.hist(PDF_Er,bins = np.linspace(0.6314,0.6824,181))
```

```
plt.title(r"$E_r\; vs\; frequency$")
plt.xlabel(r'$E_r\; {V}^{-1}$')
plt.ylabel(r'$frequency$')
plt.show()
print(f"Er is a uniform distribution with mean:{PDF_Er.mean()} V and \\
    standard uncertainity:{PDF_Er.std()} V")

PDF_Nr = PDF_dG*PDF_Er/(PDF_dH*PDF_Ei)
plt.hist(PDF_Nr,bins = np.linspace(0.3719,0.4088,2000))
plt.title(r"$Real\;efficiency,\eta_R\; vs\; frequency$")
plt.xlabel(r'$Real\;efficiency,\eta_R$')
plt.ylabel(r'$frequency$')

print(f'The resultant distribution of real efficiency has a mean of \\
    {PDF_Nr.mean()} and standard uncertainity of {PDF_Nr.std()}')
PDF_Nr.sort()
ll = int(((2.5/100)*N)-1) #lower limit
ul = int(N - ((2.5/100)*N) - 1) #upper limit
print(f"The coverage interval for 95% confidence is ({PDF_Nr[ll]}, \\
    {PDF_Nr[ul]})")


plt.axvline(x=PDF_Nr[ll],color = 'r')
plt.axvline(x=PDF_Nr[ul],color = 'r')
plt.show()
```

5 Uncertainty Estimation using GUM framework

In this section the mean and standard uncertainty is estimated using propagation of uncertainty approach according to GUM framework. Mean of measurand variables are considered as reference.Mean of and standard uncertainty of input variables are estimated from Table 1.

Table 2: Measurand Statitical Details

Input Source	Mean(μ)	a	Standard Uncertainty (u)
Gibbs Free Energy ΔG	236.2 kJ/mol	0.2	$\frac{0.2}{\sqrt{3}}$ kJ/mol
Enthalpy of formation ΔH	284.2 kJ/mol	0.6	$\frac{0.6}{\sqrt{3}}$ kJ/mol
Ideal Voltage E_I	1.3995 V	0.0105	$\frac{0.0105}{\sqrt{6}}$ V
Real Voltage E_R	0.65715	0.02535	$\frac{0.02535}{\sqrt{3}}$ V

Now the sensitivity coefficients each input variable is estimated from Taylor series expansion as

$$\begin{aligned} C_{\Delta G} &= \frac{\mu_{E_R}}{\mu_{\Delta H} * \mu_{E_I}} \\ &= 0.00165221871 \end{aligned} \tag{2}$$

$$\begin{aligned} C_{\Delta H} &= \frac{\mu_{\Delta G} * \mu_{E_R}}{\mu^2_{\Delta H} * \mu_{E_I}} \\ &= 0.5938584178 \end{aligned} \tag{3}$$

$$\begin{aligned} C_{E_I} &= \frac{\mu_{\Delta G} * \mu_{E_R}}{\mu_{\Delta H} * {\mu_{E_I}}^2} \\ &= 0.001373166993 \end{aligned} \tag{4}$$

$$\begin{aligned} C_{E_R} &= \frac{\mu_{\Delta G}}{\mu_{\Delta H} * \mu_{E_I}} \\ &= 0.278852 \end{aligned} \tag{5}$$

Now the combined standard uncertainty is given by

$$\begin{aligned} u &= \sqrt{C_{\Delta G} * u(\Delta G)^2 + C_{\Delta H} * u(\Delta H)^2 + C_{E_I} * u(C_{E_I})^2 + C_{E_R} * u(C_{E_R})^2} \\ &= 0.00878837707616392 \end{aligned} \tag{6}$$

The number of effective degrees of freedom is infinite because all the input sources are uncertainties of type B. Consequently, for a cover- age probability of 95%, the coverage factor obtained from a t-distribution is k = 1.96.

6 Results and Discussions

Monte Carlo Simulation was run using 200000 trials for the model dictated by Eq. 1 and input variables described by Table 1. The final histogram representing the possible values for the real ef- ficiency of the cell is shown on Figure 8. The resultant PDF resembles to a normal distribution.

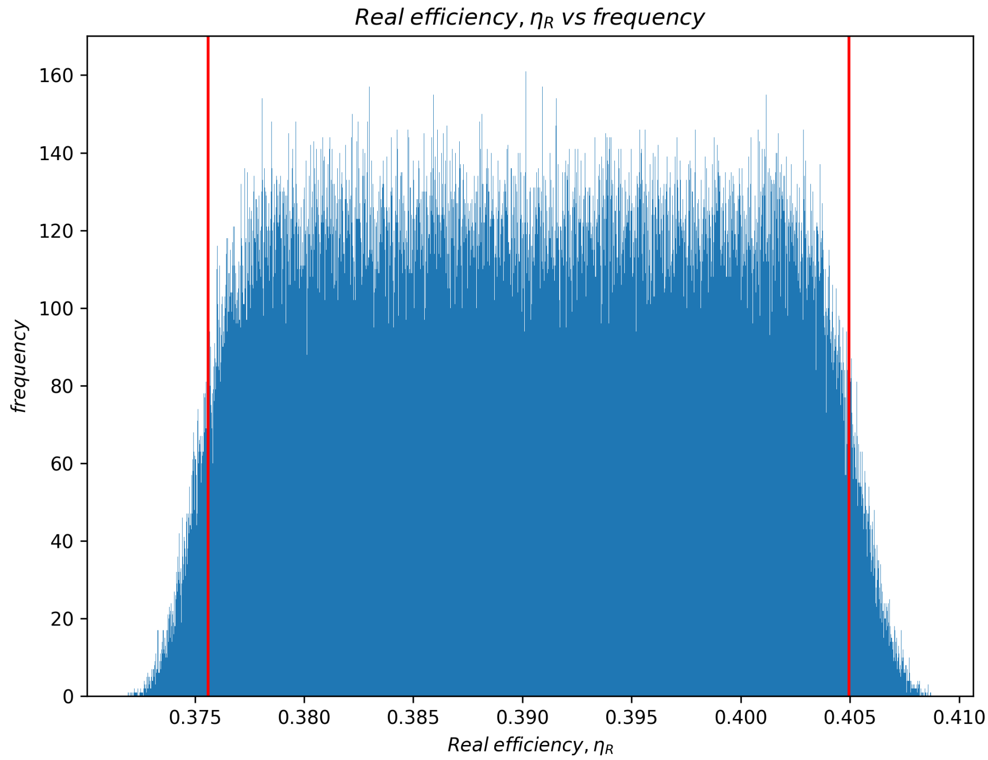

Figure 8: Histogram representing the resulting PDF for the real efficiency of a fuel cell estimated by Monte Carlo simulation

Table 3 shows the statistical parameters obtained for the final PDF corresponding to the histogram.

Table 3: Statistical parameters obtained for the Monte Carlo simulation of the real efficiency estimation model

Parameter	Value
Mean	0.390219773798723
Standard deviation	0.008776644170341664
Low endpoint for 95%	0.37562842658651535
High endpoint for 95%	0.40492047063903513

The results obtained through GUM propagation of uncertainty approach is given in Table 4.

Table 4: . Results obtained for the real efficiency of a fuel cell uncertainty estimation using the GUM uncertainty approach, with a coverage probability of 95%

Parameter	Value
Mean	0.390254
Standard deviation	0.00878837707616392
Low endpoint for 95%	0.37302878093071873
High endpoint for 95%	0.40747921906928125

It is clear from the Table 3 and Table 4 that the MCS and GUM uncertainty framework results are very close to each other.