diffraction vs. microscopy for particle sizing

AUTHOR
k. wodehouse

PUBLISHED
April 3, 2025

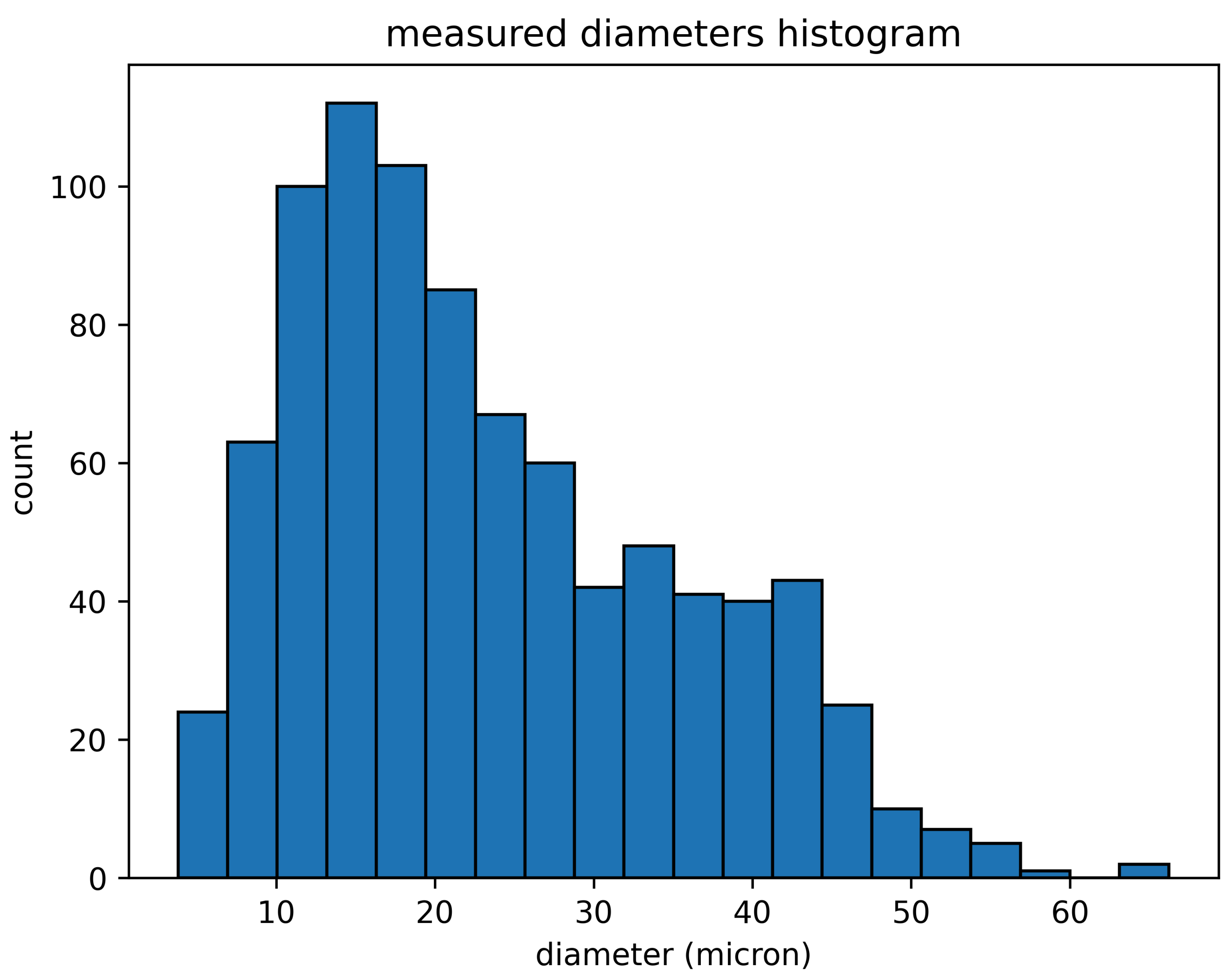
to accompany my email sent on 4/3/2025.

```
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np

df = pd.read_csv('mhec31_diameters.csv', header=None)
```

previously collected diameters

```
x = np.array(df[0])
fig,ax = plt.subplots(dpi=600)
plt.hist(x, edgecolor='black', bins=20);
ax.set(title='measured diameters histogram', xlabel='diameter (micron)', ylabel='count');
```



the average diameter using our diameter list is

```
print(f'avg. diameter: {x.mean():.2f}um')
```

```
avg. diameter: 23.49um
```

now if we use the volume fractions as weights

```
volumes = (4/3)*np.pi*(x/2)**3
vfrac = volumes / volumes.sum()
print(f'volume weighted avg. diameter: {np.dot(x, vfrac):.2f}um')
```

```
volume weighted avg. diameter: 38.66um
```

our thought experiment: 1 1m bead, 99,999 1um beads

```
beads = np.ones(1000000)
beads[0] = 1e6

volumes = (4/3)*np.pi*(beads/2)**3
vfrac = volumes / volumes.sum()
print(f'volume method: {np.dot(beads, vfrac):.6f}um')
print(f'diameter method: {beads.mean():.6f}um')
```

```
volume method: 999999.999999um
diameter method: 1.999999um
```

random sampling

now if we randomly sample from a normal distribution with the statistics computed from the microscopy

using 800 random samples (essentially our sample size)

```
beads = 11.86*np.random.randn(800) + 23.49
volumes = (4/3)*np.pi*(beads/2)**3
vfrac = volumes / volumes.sum()

print(f'volume weighted: {np.dot(beads, vfrac):.3f}')
print(f'diameter mean: {beads.mean():.3f}')
```

```
volume weighted: 35.381
diameter mean: 23.332
```

now if we do like 100,000 beads randomly sampled

```
beads = x.std()*np.random.randn(100000) + x.mean()
volumes = (4/3)*np.pi*(beads/2)**3
vfrac = volumes / volumes.sum()

print(f'volume weighted: {np.dot(beads, vfrac):.3f}')
print(f'mean: { beads.mean():.3f}')
```

```
volume weighted: 36.332
mean: 23.535
```

and these line up pretty well with what we calculated earlier just based off the diameters from the microscope. now the question becomes like why are we only seeing this with this sample? why did the other ones reasonably line up?

mhec27

let's look at mhec27 (just taking the mean and standard deviation from the email i sent march 13th and doing 100,000 random samples)

```
beads = 6.49*np.random.randn(100000) + 21.71
volumes = (4/3)*np.pi*(beads/2)**3
vfrac = volumes / volumes.sum()

print(f'volume weighted: {np.dot(beads, vfrac):.3f}')
print(f'mean: { beads.mean():.3f}')
```

```
volume weighted: 26.693
mean: 21.719
```

we can see these are much closer. and this is because the standard deviation on this sample is roughly 2x smaller than that of MHEC31. this is complete conjecture, but it could be related to the reaction vessle being switched after MHEC27.

tldr: mhec27 lines up a better since the standard deviation of the diameters is smaller by roughly 2x.

conclusion

I think a reasonable takeaway is that if we want microscopy measurements to line up more with the laser diffraction (since the whole purpose of us trying to use microscopy is to get the same results but faster) it would be a good idea to make sure we're capturing the larger particles and not worrying about the fines since their volume fractions are so small they will not affect the average much for the volume weighted/laser diffraction method, but will affect our direct diameter average.

```
# filler text, ignore this.
```