

Development of a Mathematical Model To Estimate Droplet Size Distribution of a Pressurised Metered Dose Inhaler in the Near-Orifice Region

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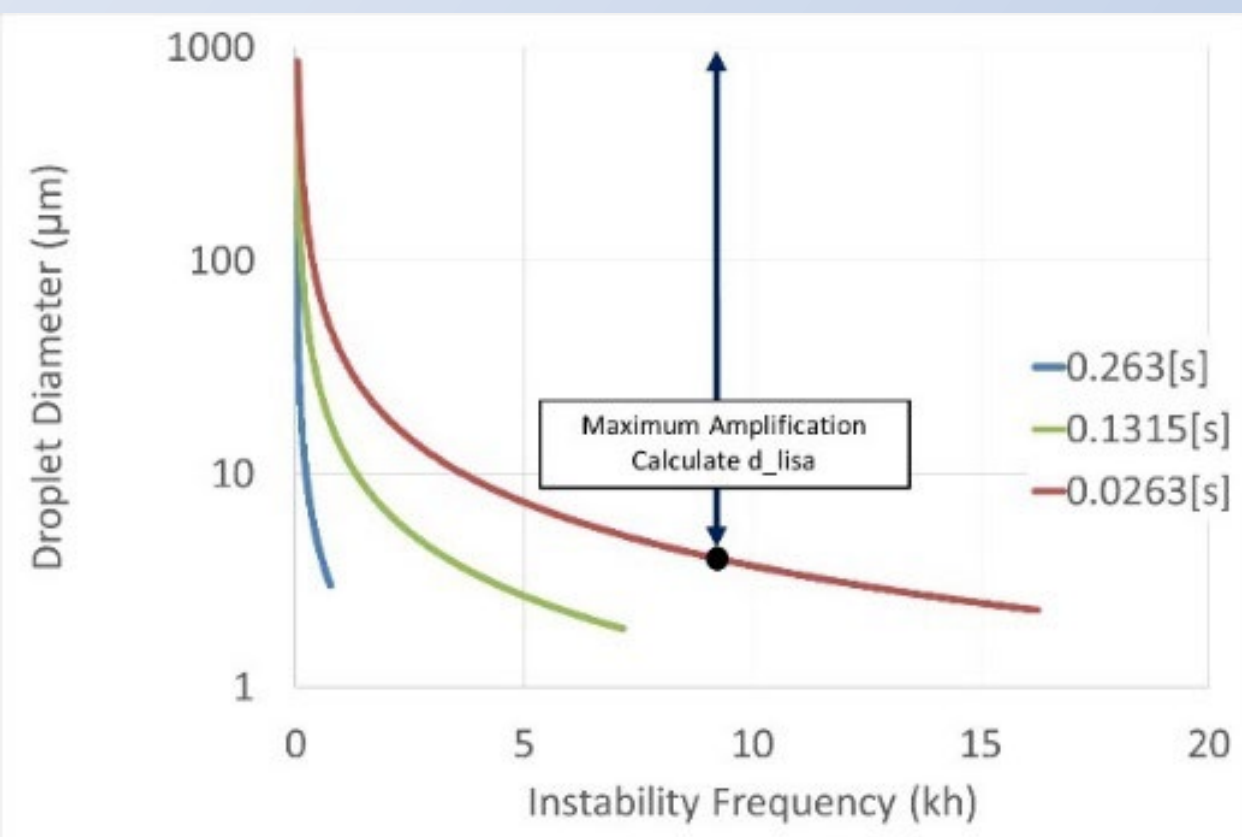
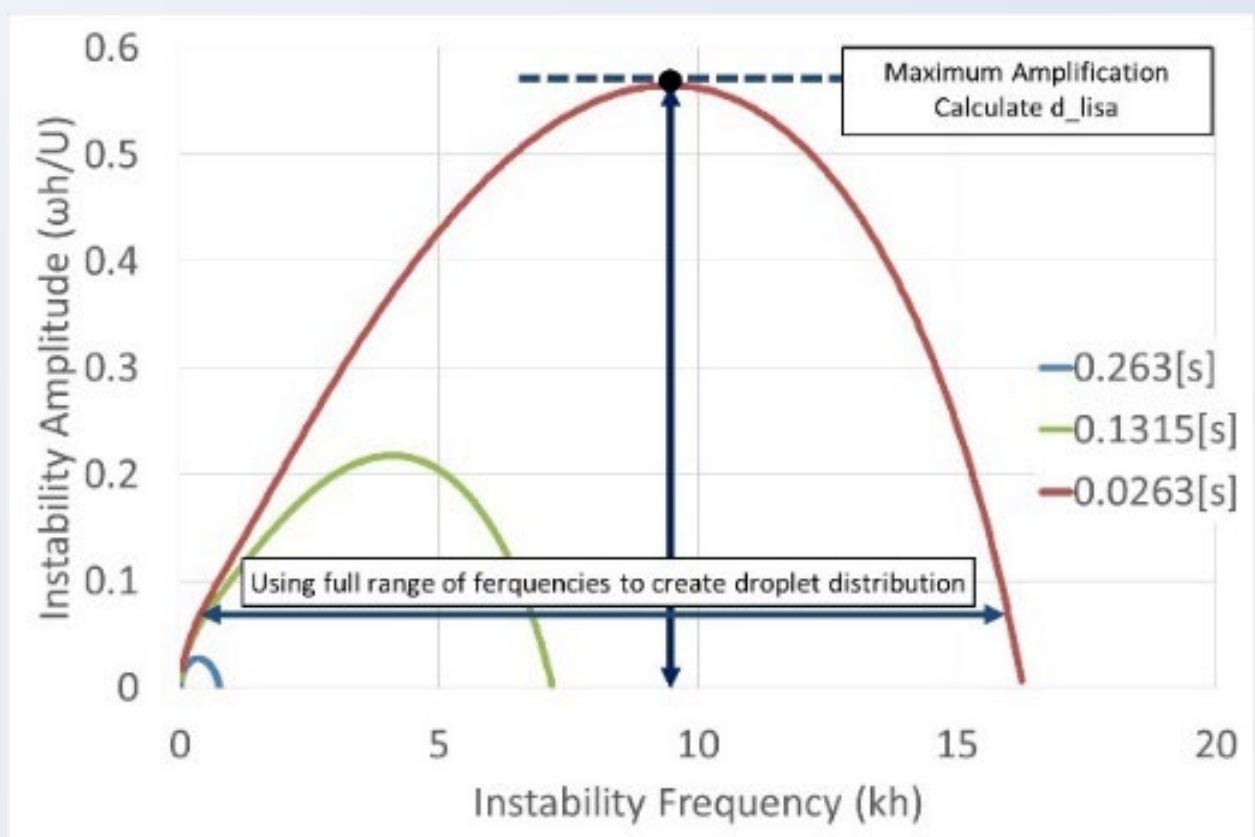
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Introduction

- Mathematical modeling and digital engineering are moving into respiratory drug delivery.
 - Experimental testing becomes very expensive.
 - More information can be gathered from a verified mathematical model.
- Computational Fluid Dynamics can be used as well, however, full CFD is still a huge challenge.
- The thermo-fluid model has the potential to mimic what is happening and at the same time, it is not too complicated/time-consuming.
- There are two main limitations to a thermo-fluid model,
 - It does not predict the spread of the aerosol distribution.
 - It will not predict what will happen outside of a pMDI.
- In this paper we will propose an improvement to the model by predicting the droplet size distribution generated by pMDI.

Method

- Assuming the atomization of the spray orifice in a pMDI is aerodynamic.
- Atomization steps:
 - Liquid surface instabilities.
 - Wave from because of the speed difference between phases
 - Stronger waves will form ligaments
 - Followed by Rayleigh instabilities ligaments form droplets
- The most amplified frequency will be the most likely droplet size generated.
- The new approach is to consider a range of instabilities around the maximum amplified frequency.
- Thus, a distribution of droplets can be generated.



- The left figure shows the estimate of different wave amplitudes for each instability frequency. Note that in our previous model the instability frequency corresponding to the maximum amplification was used to calculate the instantaneous mean droplet size droplet [8].
- The right figure illustrates the associated droplet size for each frequency.

Calculation Steps

- The instantaneous droplet size is assumed to have a log-normal distribution,

$$p(d) = \frac{1}{\sqrt{2\pi}(\ln \sigma)d} e^{-\frac{1}{2} \left(\frac{\ln d - \ln d_a}{\ln \sigma} \right)^2} \quad (1)$$

- Estimating the standard deviation from the two extreme conditions of the flow in the spray orifice.
- Calculate the probability spectrum for each possible droplet size from Eq. 1. Then, the number of each droplet size will be the normalized probability, hence,

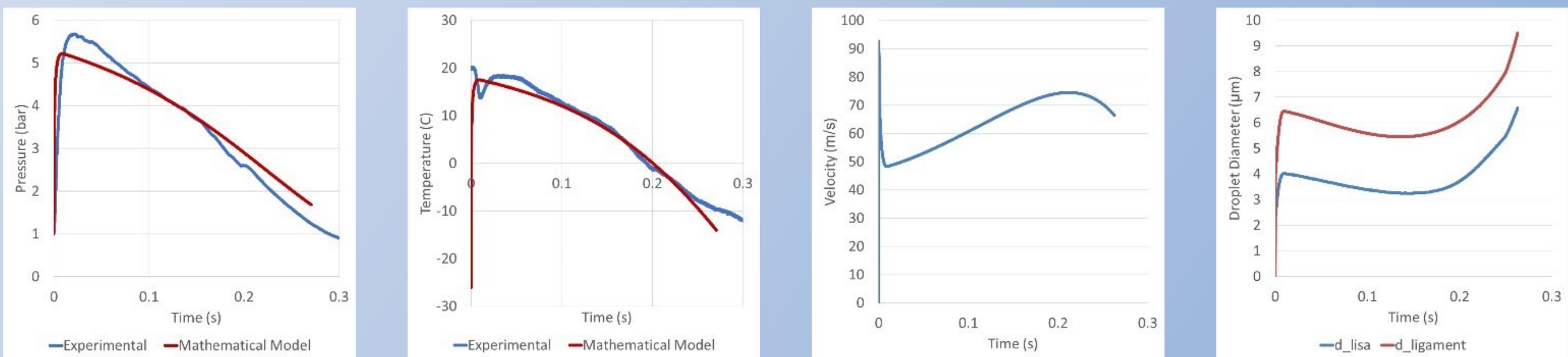
$$\overline{n(d)} = \frac{p(d)}{\sum_d p(d)} \quad (3)$$

- Find the mass for each droplet and the total mass.
- Normalize the calculated mass with the mass coming out of the spray orifice and then normalize the number of droplets accordingly.

Results (internal flow)

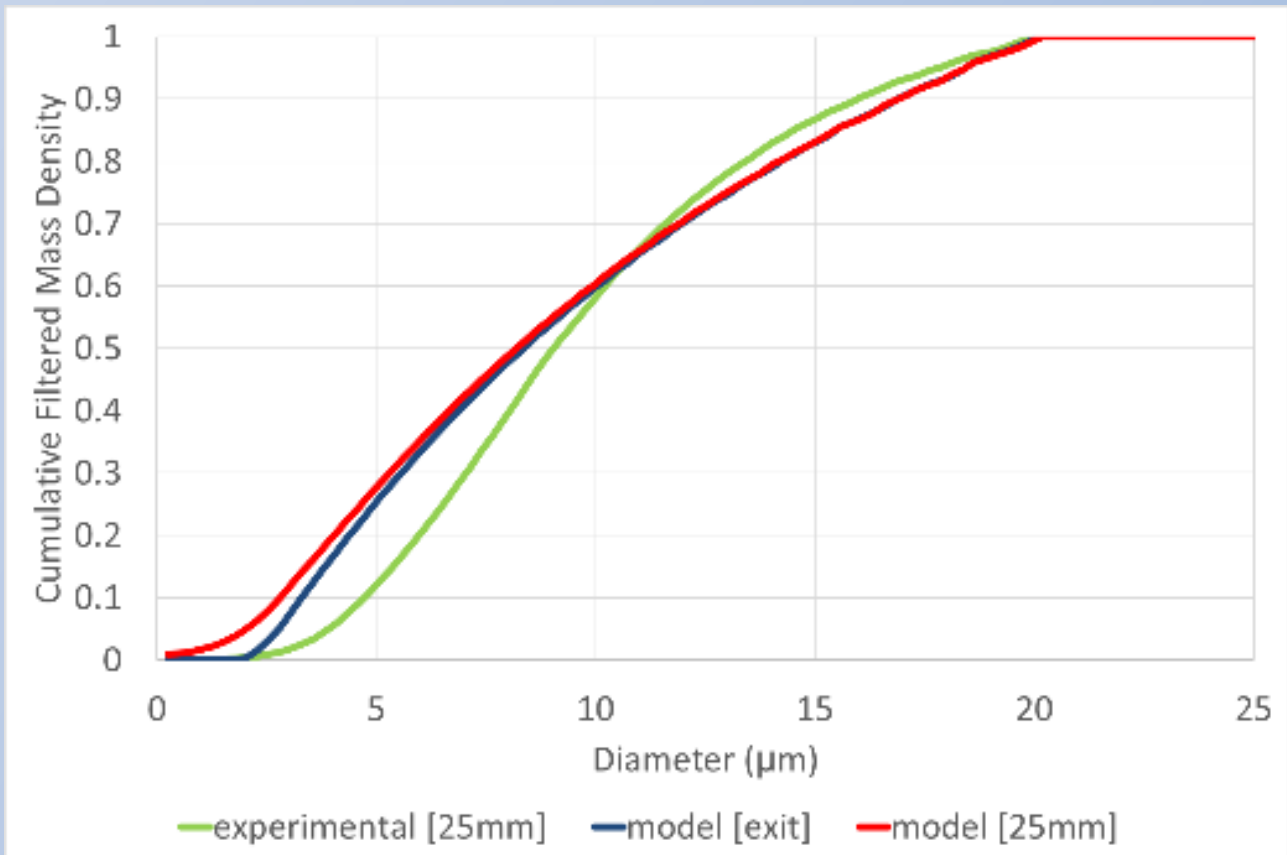
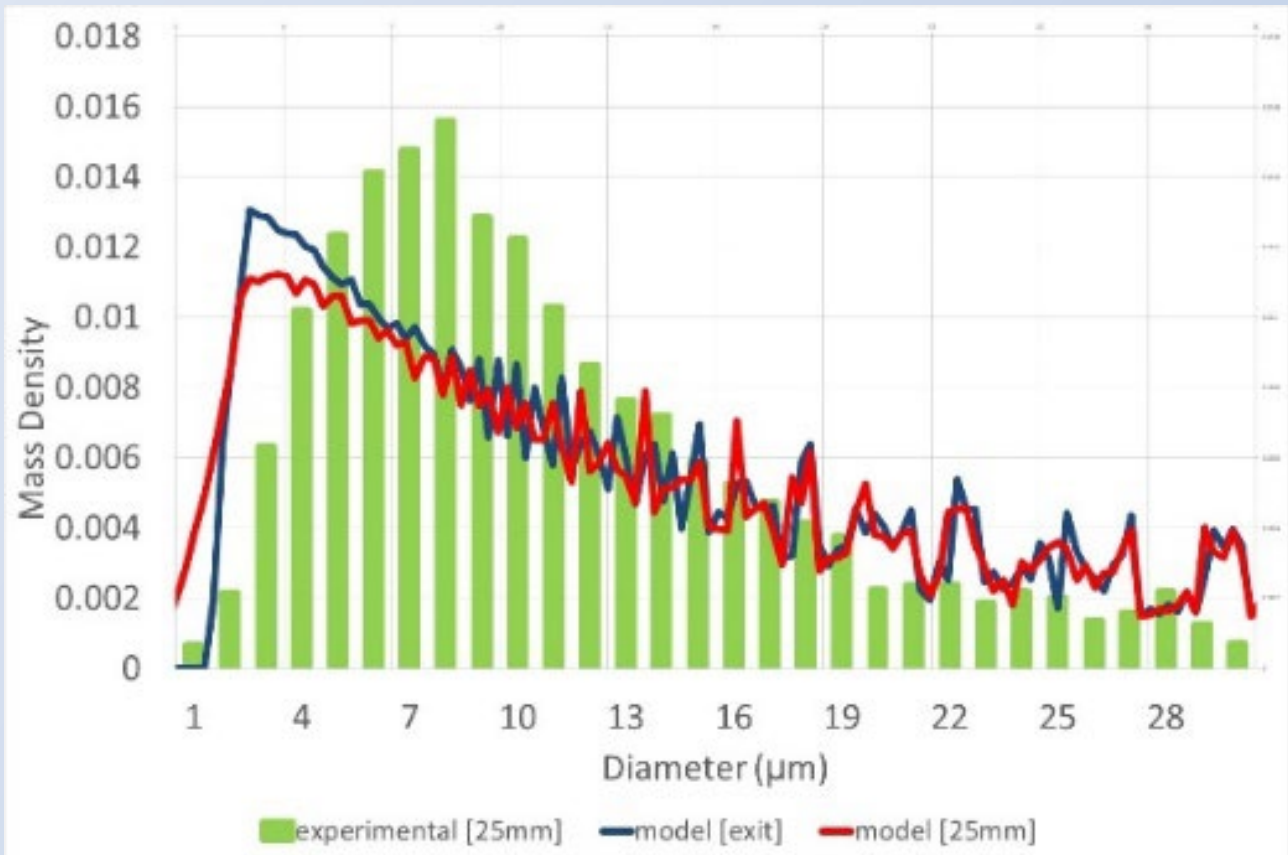
- Model results are generated for an actuation event of a test case with the following pMDI actuator parameters.

Propellant	HFA134a
Metering Chamber Volume	50 mm ³
Valve Orifice Diameter	0.62 mm
Expansion Chamber Volume	24.6 mm ³
Spray Orifice Diameter	0.30 mm



- The three figures show the computed and experimental results of expansion chamber pressure and temperature and the spray velocity at the orifice exit, respectively, as a function of time.
- The right figure shows the predicted minimum and maximum instantaneous drop diameters.

Results (external flow - droplet distribution)



The left figure:

- Illustrates the mass density of the spray droplet distribution.
- The green bars show aggregated and classified PDA data [10] at an axial distance of 25mm from the spray orifice exit.
- The two solid lines show the results from the proposed model in this study (blue = spray orifice exit; red = 25mm with the account of evaporation).
- The predicted spread of the droplet size distributions agrees reasonably well with experiments, except that the mode of the experimental mass density is at a higher droplet size than the values predicted by the model.

The right figure:

- Shows the cumulative distribution of mass density filtered to remove droplets larger than 20 microns.
- The cumulative distribution of droplets predicted by the model at 25mm of the spray orifice shows a similar d50 to the experimental measurements, but the droplet content < 1-2 µm is over-predicted.
- More precise accounts of momentum transfer and evaporation would enable us to improve these predictions.

Parameter	Experimental (PDA) [25mm]	Model [exit]	Model [25mm]
Mass d ₅₀	15.43	18.17	18.03
Mass d ₅₀ (filtered at 20 µm)	9.04	8.36	8.19
Mass d ₁₆	1.48	2.26	0.90
Mass d ₈₄	6.73	4.77	4.45
GSD	2.13	1.45	2.22
Mass d ₁₆ (filtered at 20 µm)	5.50	3.95	3.54
Mass d ₈₄ (filtered at 20 µm)	14.28	15.27	15.22
GSD (filtered at 20 µm)	1.61	1.97	2.07

- The mass d16, d50, d84, and GSD are shown for the filtered data and full data. The predicted GSD at 25 mm is stable after implementing the momentum transfer and the evaporation model.

Conclusion

- In this paper, we have improved the atomization model of Gavtash [4, 5] by including a model of the spread of the droplet size/mass distribution.
- For each time step, this model will generate a spectrum of droplet sizes. This computes the properties of the aerosol cloud produced by a pMDI and enables comparison of the numerical droplet size model directly with the experimental results of an ACI/NGI.
- The method is not limited by specific assumptions about the propellant/mixture; hence, this method can be used for any pMDI formulation for which thermophysical, and transport properties are available.

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