

## Optimization of a 2D Particle Separator – 2009

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### Abstract

**Background:** Often after a spray has been produced as a method to increase the surface area upon which a reaction can take place the byproducts of the reaction in the liquid form need to be removed from the gas phase. This project utilizes automated optimization computational design tools developed at the University of Denver to design a highly efficient spray separator with minimal pressure drop. **Methods:** Our approach is to use commercially available CFD with a Matlab<sup>®</sup>-based optimization routine and interface them together with custom coding. The optimization routine manages the CFD code by importing any number of variables within ranges and/or distributions set by the user. **Results:** We evaluated a gas-liquid separator with streamlined airfoils to maximize particle trapping, while maintaining a low pressure drop. The optimum spacing, chord length, airfoil thickness and placement were evaluated as design parameters. **Conclusions:** Our optimization routine increased the number of particles trapped while maintaining a low pressure drop for 2.5 micrometer particles.

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### Introduction

Minimal research has been done implementing numerical optimization techniques with computational fluid dynamics (CFD). CFD software packages can be complex and powerful tools used for fluid analysis and only recently, with the increase in power of computers, has it been possible to combine computational tools with optimization routines. Briefly, CFD is a technique utilized in fluid mechanics to solve complex fluid flows through the application of numerical methods and algorithms. CFD driven optimization has been explored by several researchers. One proposed a design tool that implements multi-constrained optimization of shape design driven by Genetic Algorithms (GA) coupled with CFD. The benefit to GA is that they can handle a large number (20+) of design constraints [1]. The downside to GA with a large number of constraints is that it is very computationally expensive. Peigin et. al. reports 15-18 hours for a single point optimization and on average 8-12 optimization steps. The calculation was carried out on an unknown cluster. A similar multi-constrained optimization strategy has been implemented on a ship's hull. Again the downside is the time constraints, where they report approximately 10 days for 20 generations on a PC based cluster [2]. Many researchers are using these GA in order to optimize a system with numerous constraints.

Our approach is to develop and implement a computational interface for automated design, optimization, and probabilistic analysis to a particle separator. Due to the potentially large computational times to run GA optimization, our approach is to reduce the number of constraints through probabilistic analysis in order to use single objective optimization techniques. We decided to apply this technique to novel designs for particle separators to be used within chemical lasers. Converging to an optimized design and using probabilistic analysis will therefore provide insight into the features that most affect performance, while providing the potential to reduce the manufacturing costs and weight of the total system. Additionally, manufacturing tolerances will be evaluated by probabilistic analysis providing insight into the sensitivity of geometric variables. This will in turn, reduce manufacturing costs by determining which dimensions effect the performance of the design and which geometric tolerances can be loosened. The attraction to this design tool is that it will allow for fast optimization by reducing the number of constraints through probabilistic analysis, as well as, provide insight to manufacturing tolerances, all of which is possible on readily available workstations.

We have chosen to apply our techniques in this work to the optimization of a gas-liquid spray separator. There are numerous types of particle separators used in many different applications, but there are four basic mechanisms that contribute to the separation: gravity, centrifugal force, impaction, and electromotive force [3]. Often after a spray has been produced as a method to increase the surface area upon which a reaction can take place. The byproducts of the reaction in the liquid form need to be removed from the gas phase in order to reduce downstream con-

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tamination. Wavy plate and cyclone separators dominate industrial facilities, but are frequently impractical when the active agents or excited state molecules in the gas phase have a limited lifetime requiring short residence times. This is frequently complicated by surface interactions that can quench the gas phase activity requiring further limitations on path length. Under these circumstances wavy plate separators are the classical design. These contorted designs impart significant pressure drops to the flow which can dominate pump designs and have a high surface area that can lead to high quenching. This effort specifically attempts to develop a Karbate line separator [4] design using streamlined objects to achieve high efficiency particle trapping while preserving an extremely low pressure drop.

### Materials and Methods

The computational interface software will employ sophisticated CFD codes, which solve the Navier-Stokes equations and incorporate probabilistic analysis to explore the sensitivities, importance, and manufacturing tolerances of variables within the particle separator model. Coupling all the tools together, an optimized design for the specified geometric parameters under the operating conditions was obtained. In addition to the optimized design, we can explore what parameters carry the most importance and which ones will be the most sensitive to manufacturing tolerances. With minimal effort, we can obtain results that will aid in the design process of the particle separator without needing experimental tests.

Currently, there is no commercially available tool in industry that is able to perform all the tasks mentioned above. There are however, software packages that can execute individual tasks within the automated process. The optimization routine will manage the CFD code by importing any number of variables within ranges and/or distributions set by the user. Once an optimum is found, the program will exit the routine and report the results. Figure 1 shows a simple diagram linking the processes mentioned above.

### Results and Discussion

The 2d fluid model used is shown in Figure 2. The variables that were perturbed for the optimization routine was the airfoil's location relative to the domain as well as relative to each other in the x-direction. The thickness and chord dimensions were also optimized.

The fluid modeled had an inlet velocity of 186 m/s and an outlet pressure of 50 torr. The boundary walls and airfoils were assumed to have trapped conditions. The injected particles were modeled as inert water particles with a diameter of 2.5  $\mu\text{m}$ . The number of injections was based on the size of the mesh that was automatically generated as a part of the simulation. Typically the number of injections ranged from 40 to 50. The upper and lower bounds, along with the starting points for the optimization is provided in Table 1. The objective function to minimize for the optimization routine addresses both the number of particles trapped and the change in pressure drop from a channel without any airfoils.

$$\min Fcn = 1 - \frac{p_t}{p_T} + \frac{\Delta P - \Delta P_{w/o\_airfoils}}{\Delta P_{w/o\_airfoils}} \quad (1)$$

The optimization routine had 180 total function evaluations (Fluent runs) and 10 total iterations. The final  $Fcn$  value was 0.539; where as the starting point was 0.662. Table 2 below provides the starting and final values for pressure drop and particle depositions. Figure 3 and 4 shows the pressure distributions and particle tracking for both the initial and optimized cases. The pressure distributions between the two cases differ very slightly,  $\sim 0.1\%$ , but the particle removal for the optimized case is 12.5% greater than the initial case. The optimization was performed on a HP xw8600 Workstation, running parallel on 4 processors with XP 64-bit OS and took approximately 8 hours.

From the optimized design it is critical to look at the manufacturing tolerances that may affect the design. For this analysis we will utilize Nessus<sup>®</sup>, a commercially available probabilistic software package developed by Southwest Research Institute (SwRI), in conjunction with our CFD codes. In order to set up the probabilistic analysis, we have to determine the mean values and standard deviations for each parameter. Table 3 lists these values. The standard deviations are simply the difference between the bounds divided by three. Since the design space within the typical machining manufacturing tolerances ( $\sim 0.1\text{mm}$ ) is monotonic, we have chosen to use the Advanced Mean Value (AMV) method. It has been shown that within a monotonic design space, the AMV method produces accurate results compared to the Monte Carlo method, but with a fraction of the iterations and time [5]. The result from the probabilistic analysis shows that the thickness ( $t$ ) and the distance between the airfoils ( $D1$ ) have the greatest sensitivity when perturbed and therefore should be held to a tighter tolerance during machining (Figure 5). The chord and

location (D2) of the airfoils do not affect the outcome as much and therefore tolerances can be loosened resulting in possible time and cost savings during the manufacturing process.

We validated our particle tracking CFD code with results from Pui et. al. (1987). Their paper reports the deposition efficiencies for various Reynolds and Stokes numbers within bends of a circular cross section tube [6]. Our CFD codes matched very well with the experimental results. The determining factor for the accuracy of CFD code was the inlet velocity profile. In order to have a reasonable computational time, we only modeled the bend of the tube and coded a velocity profile at the inlet. The comparison of results is presented in Table 4.

We have presented a new and novel process to evaluate and design fluid systems utilizing automated design tools that can be readily available and require reasonable computational times. Rather than using a large system of variables and GA, we have developed a way to reduce the amount of variables by probabilistically evaluating the design space and using the important constraints within the optimization routine.

## Acknowledgement

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## Nomenclature

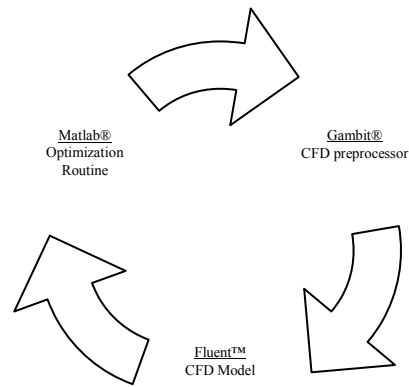
$Fcn$	function value
$P$	pressure
$p$	particle

### Subscripts

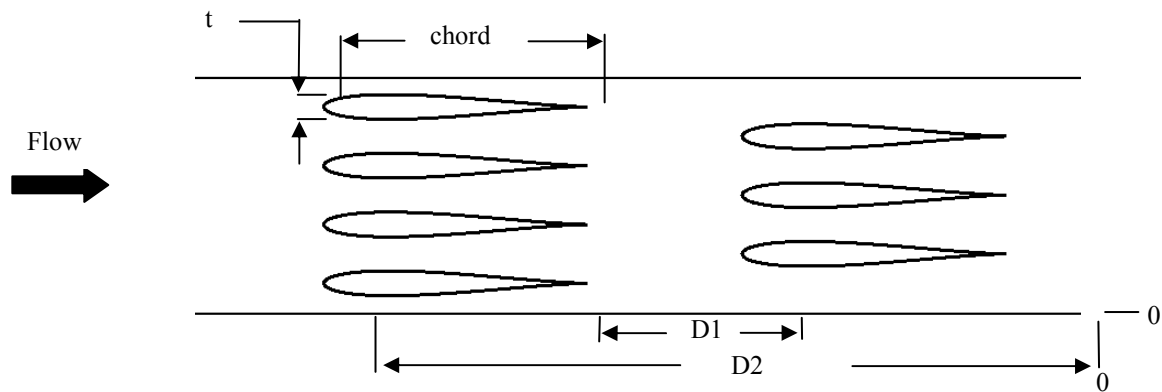
$T$	total
$t$	trapped
$w/o\_airfoils$	without airfoils

## References

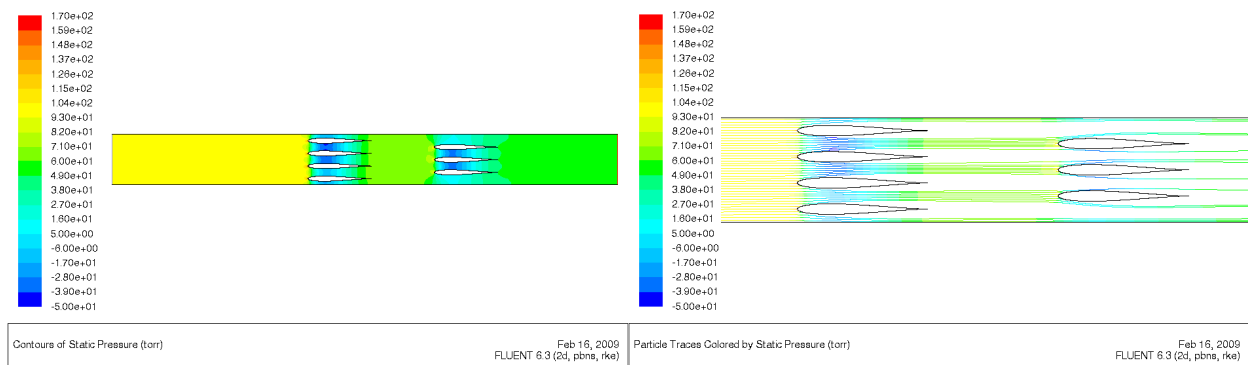
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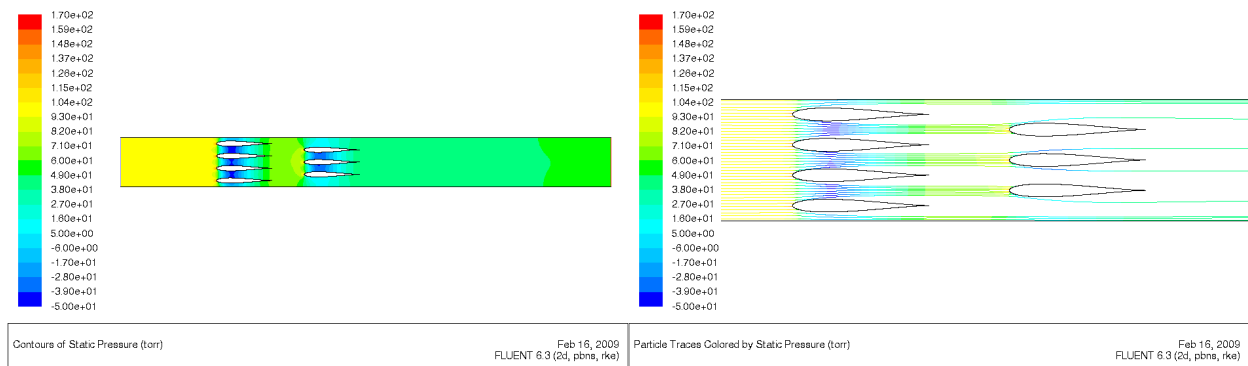
**Figure 1.** Diagram of the Optimization and CFD interface. Each program is linked by custom scripts.



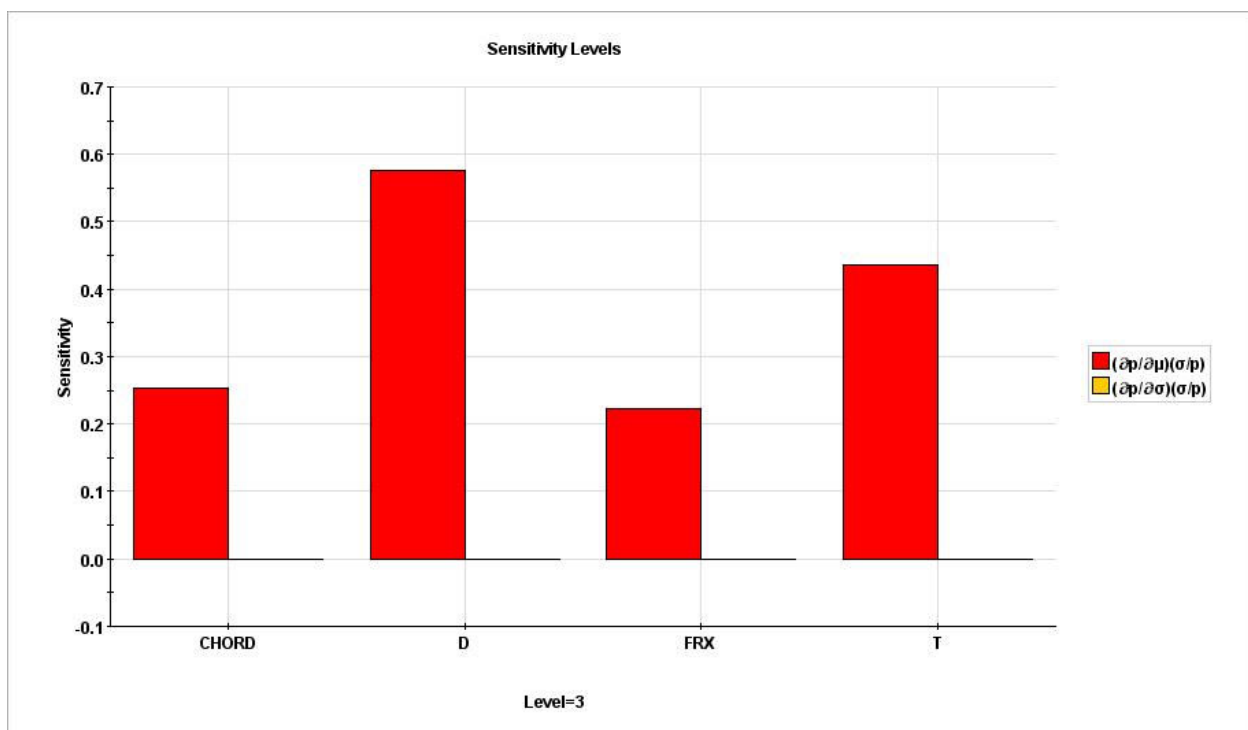
**Figure 2.** Schematic of fluid domain with airfoil particle traps to be optimized.



**Figure 3.** Pressure and particle tracking plots of the initial case of the optimization routine.



**Figure 4.** Pressure and particle tracking plots of the optimized case.



**Figure 5.** Importance Levels for the parameters perturbed.

**Table 1.** Values for the optimized variables.

	Chord (mm)	t (mm)	D1 (mm)	D2 (mm)
Starting Point	5.000	0.400	5.000	-2.000
Lower Bounds	1.000	0.100	1.000	-15.000
Upper Bounds	7.000	0.730	5.000	0.000
Optimized Point	4.502	0.422	2.645	-9.920

**Table 2.** Values for initial and optimized simulations.

	Pressure Drop (torr)	Particle Deposition (trapped/total)	Fcn
Starting Point	72.06	25/40	0.662
Optimized Point	72.17	30/40	0.539

**Table 3.** Table of the mean and standard deviation values entered into Nessus<sup>®</sup>.

Variable	Mean	Std. Dev.	Distribution
Chord (mm)	4.502	0.833	Normal
t (mm)	0.422	0.1	Normal
D1 (mm)	2.645	0.75	Normal
D2 (mm)	-9.920	1.75	Normal

**Table 4.** Table of the comparison to validation case.

Case	Re	St	Experimental Depo- sition efficiency (Pui, et. al.)[6]	CFD Deposition Efficiency
1	1000	0.17	5.3	2.1
2	1000	0.28	24.5	24.9
3	1000	0.33	37.7	37.7