Optimization of an explosive trace detector using CFD simulation

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The VOLPE project aims to provide a solution to the growing demand for innovative security systems for early prevention and response. The aim of the project is to design, develop, and optimize a completely contactless explosive trace detector to continuously monitor dangerous and hazardous volatile compounds in the air to safeguard both citizens and critical infrastructure.

These substances are particularly difficult to monitor because they are constantly changing and improving, often being created from bare precursors, i.e. common substances that only become harmful when mixed e.g., fertilizers, fuel, and bleach. There is, therefore, a growing need for smart detection devices that can simultaneously monitor multiple chemicals and process complex correlation analyses from large raw datasets.

The project aims to develop a sensor system for the detection of volatile explosive substances, capable of continuously monitoring the air without the presence of an operator. Currently, checks for explosive substances are carried out with instruments based on buffer systems that require the presence of an operator and a sample check.

The possibility of checking all samples without the presence of an operator makes this type of technology very attractive, and it could find many other applications, such as checking postal packages, people or other sensitive venues. The final product is designed to increase the number and effectiveness of security checks within critical infrastructures, such as embassies, museums, shopping centres, post offices, etc. A pre-industrial prototype of this tool has already been successfully implemented in previous projects (SPECTRE, EXIN), and its functions have been tested in a real environment at the Marco Polo airport in Venice. The positive outcome of these experiments prompted the desire to continue with the industrialization phases of the prototype, with the aim of creating a version compatible with market requirements.

Fig. 1 - Baggage moving on the conveyor belt under the prototype.

The VOLPE project was funded by the Veneto Region of Italy under the “POR FESR 2014/2020 Asse 1 Azione 1.1.4” programme and was developed in partnership by three companies: EXA, EnginSoft and Buson. Thanks to the shared efforts of the companies, an engineered and fully automated prototype has been created. The prototype consists of:

- an automated system capable of controlling both a conveyor belt for handling luggage and a translation system that adapts the position of the detection system to the different heights of the luggage;
- an air system capable of drawing air from the baggage and conveying the sample to the detection system;
- an optoelectronic detection system, consisting of: a reaction chamber where the air sample is conveyed; an optical sensor that varies its optical properties in the presence of the target molecules; and an optoelectronic system for signal acquisition.

This article will focus on the numerical computational fluid dynamics (CFD) simulations developed by EnginSoft to support the performance optimization and component miniaturization of the air suction system.

Case Study

The optical nanotechnology on which the sensor system is based has demonstrated the necessary performance for the detection of traces of explosives. EXA is currently the exclusive licensee of two patents (Application No. IT2016UA02589 20160414 and IT2016UA02587 20160414, owned by ARC-Centro Ricerche Applicate, EXA’s partner) for the industrial production of optical devices, which are part of the sensor system in question.

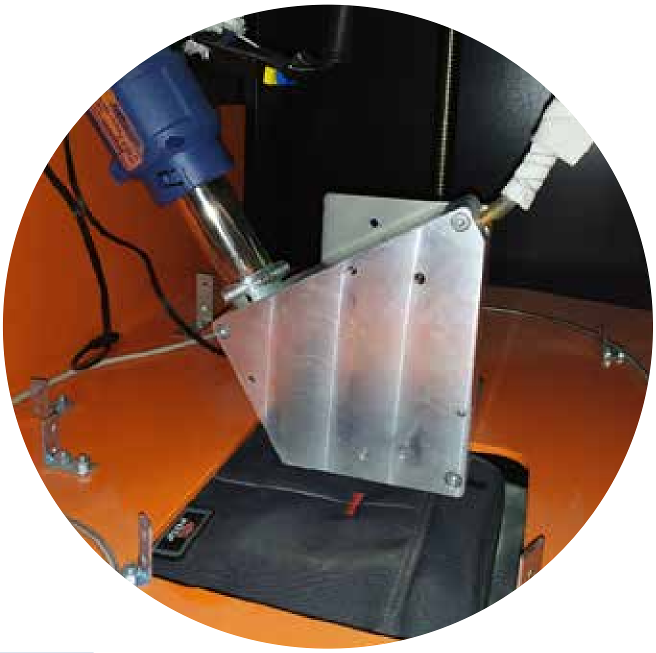

Fig. 2 - Internal part of the prototype, consisting of the heat gun on the left and the aspiration duct on the right.

The system under analysis is illustrated in Figs. 1 and 2, which show the first prototype of the detection system. The prototype is mounted on a conveyor belt, on which the suitcase can move. It includes a heat gun, which delivers 8.5 l/min of air at 450°C or 600°C to the moving luggage. There are then two aspiration ducts, one is connected to the heat gun via a nozzle, the second is connected to the measuring cell to collect molecules. The flow of 36 l/min is guaranteed by a constant flow pump.

Numerical simulations were performed in four phases. In the first step, a mathematical model was developed to reproduce the behaviour of the actual prototype, in order to calibrate the configuration of the experimental data. EXA provided a complete characterization of the functional behaviour of the prototypes, using a custom-developed test bench capable of investigating the correlations between all relevant system variables.

The second activity focused on the identification of the most relevant parameters, which led to the third step, the implementation of a parametric CFD model. Finally, these parameters were used to modify the device with a view to optimizing the design and identify an improved prototype. This last step was repeated along with experimental tests to support the numerical results and guide the optimization roadmap, so two prototypes were identified and tested consecutively.

This procedure had the following objectives:

- Optimize the fluid-dynamic characteristics of the intake air fraction
- Assess and improve baggage coverage
- Ensure the best temperature control
- Reduce cost components and energy consumption
- Minimize device size

Modelling approach

The numerical model was built using the Ansys suite to reproduce the experimental setup and then to optimize the device. The starting points were the 3D CAD geometry and the data obtained from experimental tests, which provided information on both the geometrical parameters and the operating conditions.

To simulate the aspiration system, it was not necessary to consider the complete prototype, but instead to focus on the details between the luggage, the heat gun, and the aspiration duct. Since the geometry was symmetrical, the computational domain was split in half with respect to the conveyor belt.

The fluid domain was extracted starting from the 3D CAD of the solids. De-featuring was used to simplify and remove details that were not relevant for fluid dynamics and could be neglected. Bodies and volumes were split to simplify the subsequent meshing procedure and to set up different physics.

The suitcase was simulated as a 2 mm thick solid, placed at a distance of 5 mm from the aspiration system, with a prescribed translational speed. The computational domain around the component (Fig. 3) was extended in three directions to consider an air plenum around the area of interest. Therefore the volume had an extension of 1 m in the direction of the belt, 0.2 m in the lateral direction and 0.2 m in the vertical direction. The air ducts, which are connected to the heat gun and the pump, were extended to stabilize the fluid flow at the boundary conditions.

To solve the CFD analysis, the geometrical model was discretized into a computational grid. The mesh was generated with an adequate cell size to evaluate local physics phenomena with good resolution. Prisms were constructed at the walls to correctly capture the boundary layer where high velocity gradients occur. Quality criteria were checked to reduce element distortion and ensure valid results. The mesh generated in Ansys Fluent Meshing

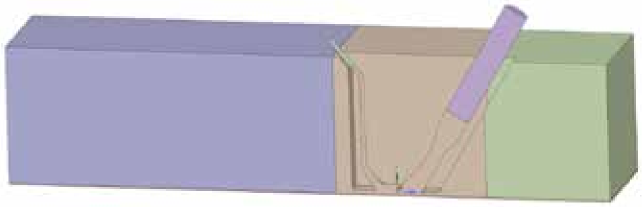

Fig. 3 - Computational domain.

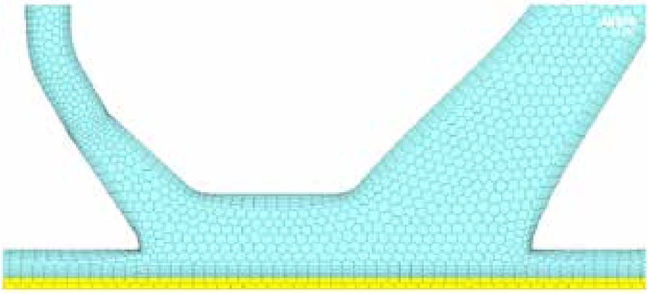

Fig. 4 - Detail of the polyhedral mesh on the symmetry plane.

Physical properties of materials	
AIR	
Density	Ideal Gas
Viscosity	1.7894E-5 [kg/ms]
Specific heat capacity	1006.43 [J/kgK]
Thermal conductivity	0.0242 [W/mK]
Molecular weight	28.966 [kg/kmol]
POLYSTYRENE	
Density	1045 [kg/m3]
Specific heat capacity	1249 [J/kgK]
Thermal conductivity	0.12961 [W/mK]

Table 1 – Material properties

REGION	BOUNDARY CONDITIONS	
HEAT GUN	Boundary type	Inlet
	Q [l/min]	8.5
	T [°C]	450 – 600
ASPIRATION PUMP	Boundary type	Outlet
	Q[1] [l/min]	36
CONVEYOR	Boundary type	Fluid-Solid interface
	v [cm/s]	2.31 – 4.57 – 7.60
VOLUME BORDERS	Boundary type	Opening
	p [Pa]	101325
	T [°C]	26.85

Table 2 – Summary of boundary conditions

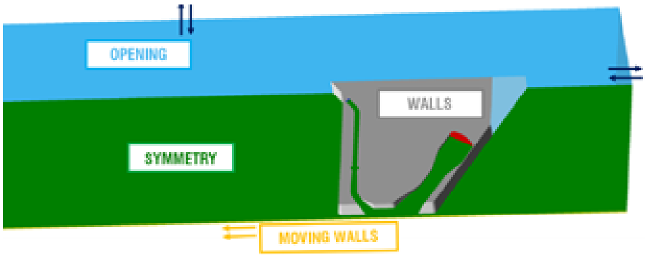

Fig. 5 - Summary of boundary conditions.

Input Parameter	Variable	Description	Range
P1	T_{gun}	Inlet temperature	450, 600°C
P2	V_{belt}	Conveyor belt velocity	2.31, 4.57, 7.6 cm/s
P3	Φ_{IN}	Diameter of the inlet duct, connected to the heat gun	2 ÷ 10 [mm]
P4	Φ_{OUT}	Diameter of the outlet duct, connected to the pump	1 ÷ 4 [mm]
P5	Q_{IN}	Inlet mass flow	0.85 ÷ 8.5 [l/min]
P6	Q_{OUT}	Outlet mass flow	3.6 ÷ 36 [l/min]
P7	α	Inclination angle of the outlet duct	15 ÷ 45 [deg]
P8	β	Inclination angle of the inlet duct	0 ÷ 45 [deg]
P9	d	Distance between inlet and outlet ducts	4 ÷ 44 [mm]
P10	H_{GUN}	Distance between inlet gully and horizontal plane	0 ÷ 40 [mm]

Table 3 – Summary of the inlet parameters

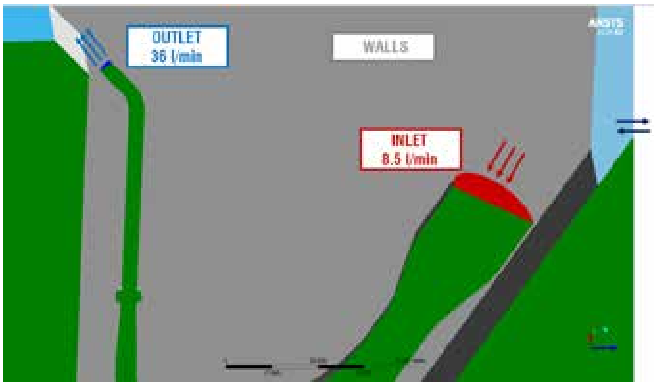

Fig. 6 - Summary of boundary conditions.

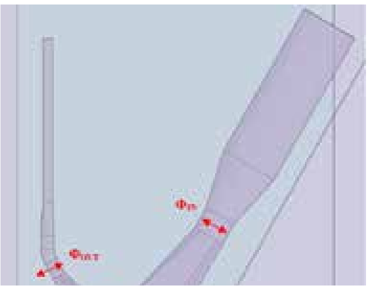

Fig. 7 - Representation of Φ_{IN} and Φ_{OUT} parameters for investigating gully shrinkage.

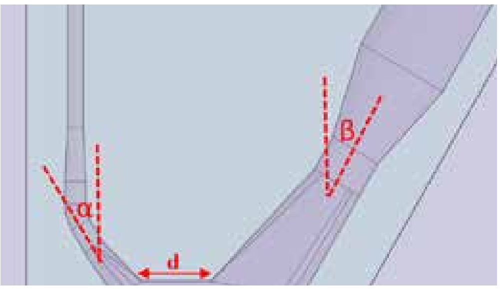

Fig. 8 - Representation of parameters α, β and d, to investigate the geometrical shape of the device.

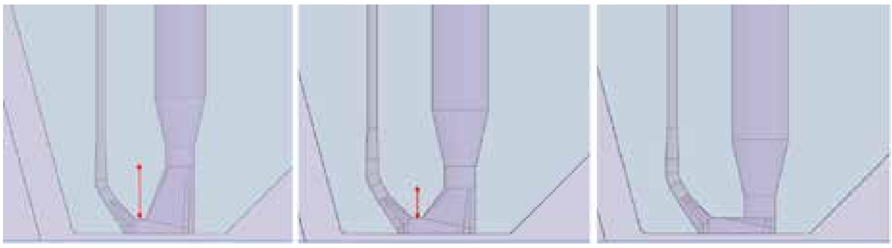

Fig. 9 - Representation of Hgun parameters, to investigate the geometrical shape of the device.

(Fig. 4) was composed of 8.7 million nodes and 1.8 million polyhedral cells.

Subsequently, the computational grid was imported into the Ansys Fluent solver, where the physical models, operating conditions, and numerical setup were defined. In particular, air was considered as an ideal gas to account for density variations. The suitcase was modelled as a polystyrene solid in conduction with the fluid. The physical properties of the materials are summarized in Table 1.

The flow considered is turbulent and the analyses were carried out in steady state, considering the physical phenomenon as fully developed.

The operating conditions, derived from the technical specification of the instruments and the EXA experimental data, are summarized in Table 2 and displayed in Fig. 5.

Exploring possible modifications of the aspiration system, several sets of parametric studies were performed, considering different input and output parameters. The input parameters represent both geometrical configurations and physical quantities. These are summarized in Table 3 and displayed in Figs. 7, 8, 9. The output parameters were set to investigate the objectives mentioned above, i.e. they are identified as follows:

- Average temperature at outlet
- Temperature distribution in the suitcase area
- Composition of the air sucked in by the pump
- Concentration of target molecules at the outlet

Results and discussion

The results made it possible to evaluate the actual performance of the system, to check parameters that had not been quantified experimentally and to improve layout performance by focusing on relevant quantities, i.e. it was possible to evaluate each flow path and determine the composition of the air sucked into the pump, passing through the measuring cell. The outlet flow is in fact a combination of ambient air and hot air from the heat gun. A correlation was found between input and output parameters, which guided the entire optimization procedure.

The following points list the main input and output considerations in order to summarize the relevant issues arising from each step of the simulation process:

- The inlet temperature (T_{gun}) is related to the temperature of the suitcase.
- The conveyor belt velocity (V_{belt}) has a limited impact on the temperature, pressure, and velocity profiles.
- The inlet diameter (Φ_{IN}) has a strong influence on the sample temperature. For smaller diameters, there is less collection of molecules because there is more dispersion of the heated air to the environment. In fact, for smaller diameter configurations, the impact with the surface is greater as the velocity increases, preventing air from being collected in the outlet duct.
- The outlet diameter (Φ_{OUT}) has a negligible impact on the output parameters considered, so it can be excluded from further considerations.
- The mass flow inlet (Q_{IN}) has a medium sensitivity, with direct correlation to temperature and suitcase coverage.
- The mass flow outlet (Q_{OUT}) is a high sensitivity parameter, with inverse correlation to temperature and suitcase coverage.
- The angle of inclination of the outlet duct, α, has a low influence, showing that the mass flow is relevant for the aspiration duct, while the diameter and inclination are not.
- The angle of inclination of the inlet duct, β, has a strong impact on the suitcase coverage and the outlet concentration.
- The distance between the ducts, d, has a strong influence on all outputs.

  A greater distance between the two ducts leads to overheating of the sample and, consequently, to a higher suction and suitcase temperature, and suitcase coverage.
- The distance between the inlet gully and the horizontal plane (H_{GUN}) does not have a major impact on the suitcase coverage, which remains unchanged when the distance between the heat-gun and the horizontal plane varies.

The simulation campaigns made it possible to conduct a product development study to identify new prototypes. In particular, the device evolved in two phases which are shown in Figs. 10, 11, 12, 13. During this procedure, the choice of new layouts was guided by the following aspects, which were selected as high priority and experimentally validated on the test bench:

- miniaturization of the device
- reduction of sample coverage
- increase of detected molecules

The reduction in area, referred to in the second point, is due to the fact that if the target molecules were restricted to a

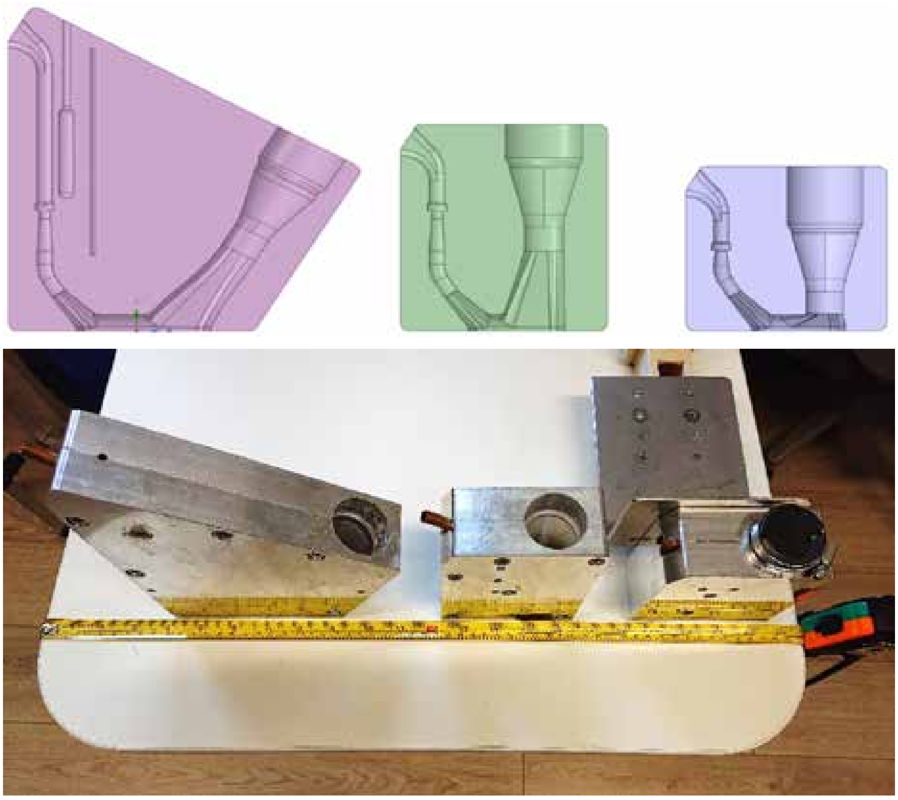

Fig. 10 - Evolution of the layout: CAD model (top), manufactured product (bottom).

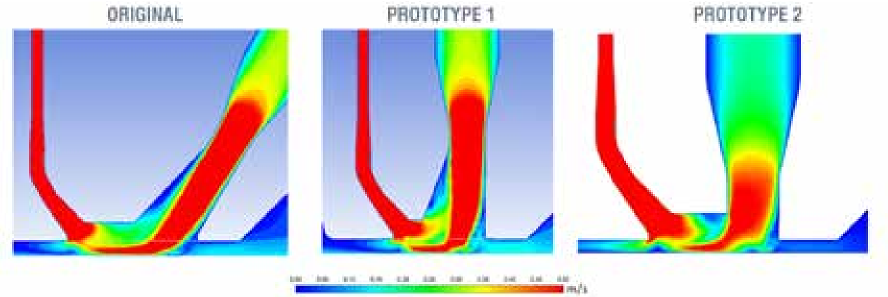

Fig. 11 - Velocity profile in three cases.

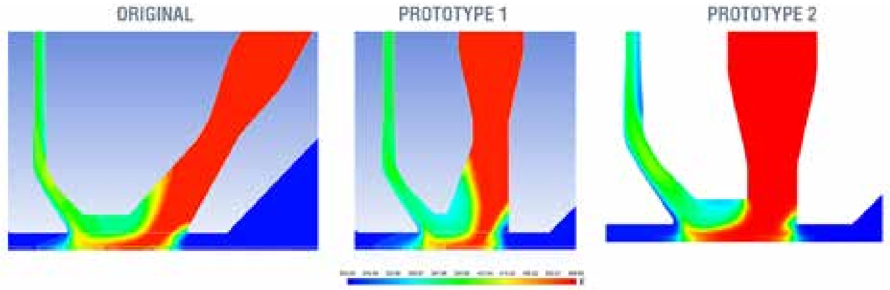

Fig. 12 - Temperature profile in three cases.

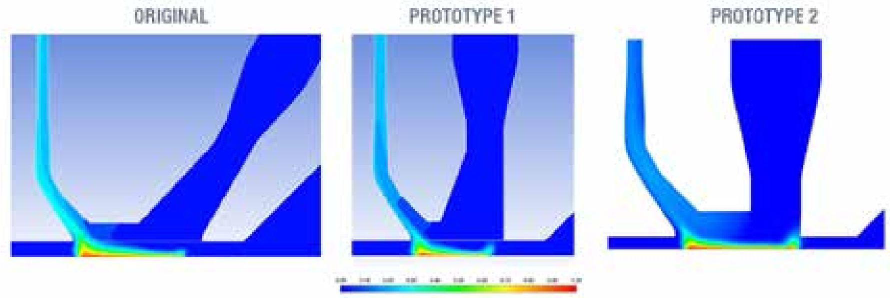

Fig. 13 - Distribution of target molecule in three cases.

limited region of high concentration, high coverage could result in excessive dilution of the air sample.

The selection of the best design minimizes the distance between the ducts (d), places the inlet duct in a vertical position, and minimizes the distance between the inlet gully and the horizontal plane (HGUN).

Conclusions and future work

CFD simulation was successfully applied to design and optimize all components of the system for the contactless detection of hazardous substances in hand luggage.

The final optimal design met the objectives and was experimentally validated on the test bench with the following KPIs:

- miniaturization of the device through the optimization of the air system in terms of the fraction of air intake compared to the luggage area analysed;
- reduction of sample coverage with optimization of sampling, thanks to a fully automated system that varies the position of the detection system according to the height of the luggage;
- an increase in the number of molecules detected by parallel detection of several molecules, through the development of a multi-spot sensor and a suitable optical system including a massive reduction of false positive results due to specific control spots incorporated into the optoelectronic sensor.

A final prototype was produced and validated in a bench test.

EXA's next main objective is to apply this technology to other sectors where security is paramount, e.g. civil security and food processing chains. This will be achieved thanks to the great versatility EXA technology, which can be applied in any situation that requires careful and reliable real-time analysis, especially on moving samples.

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About EXA

EXA is an Innovative SME established in 2016 for developing a detection system of dangerous molecules, e.g., explosives and drugs, in gas samples. This activity was based on a technology transfer process from university research results to the safety equipment market.
Based on an analysis of the characteristics and requirements of the security sector, the company developed a prototype driven by critical technology drivers: real-time analysis, operational autonomy, continuous and contactless analysis, high sensitivity and high throughput. This first prototype was installed in Venice airport for testing on hand luggage boarding checkpoints.