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Improvement of Plasma Gun Performance using Comprehensive Fluid Element Modeling: Part I

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The use of computational fluid dynamics (CFD) to model the operation of thermal-spray processes has gained interest in the thermal-spray community, able to provide an understanding as to how a process functions, and better how to make a process work better. Advancements to the science of modeling now permits the ability to create a comprehensive model of a plasma gun that not only simulates the dynamics of the gas, but also the mechanics of arcs (plasma), thermodynamics, and entrained particulates to form a nearly complete model of a working thermal-spray process. Work presented includes the methods and procedures used to validate the model to a Sulzer Metco TriplexPro^{TM}-200 plasma gun and exploration of the operating regime to give an in depth and insightful look into the physics behind the operation of a triple-arc cascaded plasma gun.

Keywords flow simulation, magneto-hydrodynamics, particulate flow, plasma spray gun, process optimization, supersonic flow

1. Introduction

Recent developments in flow simulation software, numeric modeling, and hardware make the reliable use of simulation tools for the development of spray guns in an industrial environment feasible (Ref 1). From a fluid dynamics point of view, a spray gun features many interesting phenomena, like supersonic flow, particle transport and fluid heating by arcs. The later one calls for the coupling of the plasma arc modeling with the flow models. Such a coupling goes beyond the capability of most commercial codes for computational fluid dynamics and, therefore, development of additional models is necessary. As the quality of CFD depends on numerical methods, models, parameter settings and boundary conditions, a thorough validation for any new application is absolutely necessary. Only then, the designer can trust in the CFD results and draw conclusions for the optimization of the spray gun.

The article is the first part of a two parts article and focuses on the modeling of fluid dynamics and electromagnetism and its first validation runs for the Sulzer Metco TriplexPro^{TM}-200 plasma gun. In the companion paper to this one, further applications of these tools in the industrial design environment are covered (Ref 2).

2. Simulation Models for Spray Gun Development

Classic CFD, as widely used in industry and academia, calculates the flow through or around an object of interest. The simplest case is the simulation of single-phase fluid flows, either incompressible or compressible. Flow computations use the well-known Navier-Stokes equations, which are numerically rearranged, in order to be efficiently solved by an iterative scheme. In most cases, turbulence is taken into account by using an appropriate turbulence model from a wide selection. Although turbulence could be computed without modeling by direct numerical simulation, this is not feasible for real industrial applications, as computer power is still several orders of magnitude too slow for such applications. Depending on the nature of a multiphase flow consisting of a continuous and disperse phase, it can be simulated by solving the Navier-Stokes equations for each phase (Euler-Euler method) or by a particle tracking algorithm (Lagrangian method). The latter is of interest as we consider the transport of particles through the nozzle up to the substrate. Furthermore, other physical phenomena, like plasma arcs, can be modeled as well, and need to be coupled to the standard flow simulation. Depending on the information required from a flow simulation the appropriate combination of CFD models has to be selected and, if necessary, adapted.

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The following paragraphs give a brief overview of various CFD setups of different complexity, all useful for the development of thermal spray guns. This step-by-step method was also necessary due to the complex nature of the physics in the plasma gun. Once, a step was validated, it could be used as the base for the next and more complex step.

2.1 Simulation of the Supersonic Gas-Only Flow

In the Sulzer TriplexPro$^{\mathrm{TM}}$-200 Plasma gun supersonic flow conditions exist downstream of the critical cross section in the nozzle. Therefore, such a simulation might be of use for an initial assessment of the gas dynamic performance of the spray gun. It can be run with any commercial CFD code capable of computing supersonic flow. Special care is needed in the selection of the turbulence model to predict correctly the turbulence flow structure. The heating of the fluid by the plasma arc can be taken into account by locating a heat source within the fluid domain in the area where the real arc is present. It is assumed that the heat flux is constant and no spatial variation is considered. The quantity of the heat flux has to be estimated from experimental data. Based on electrical power input and the heat removed by the cooling water, the power for the heat source can be estimated. The results of such a simulation setup can be compared to measurements taken from a spray gun being run without particles. Such a setup has been successfully used to optimize the gas inlets and chamber of the Sulzer TriplexPro$^{\mathrm{TM}}$-200 Plasma gun, see below. In this case, the area of interest is upstream of the particle feed and the arc has almost no influence on the gas flow field in the chamber.

2.2 Simulation of the Supersonic Gas Flow with Particles

The setup outlined in the previous paragraph can be augmented by including the particles. There exist two basic models of Lagrangian particle tracking. The simplest one features a one way coupling between the gas flow and the particles. The particle tracks are computed from the continuous flow field and the gas flow is not affected by the particles. This method is computationally very cheap and can be run in the postprocessing. However, it is not recommended for spray guns, as the particles get strongly accelerated by the gas flow as they are injected and therefore influence the flow field. This phenomenon can be taken into account by implementing a particle tracking model with two-way coupling, i.e., the flow influences the particle tracks and vice versa. The problem here is that the models available in the CFD codes are usually not intended for supersonic flows and, hence, the drag and heat transfer is not correctly predicted.

A friction-heating model had to be introduced to predict correctly the heat transfer between gas and particle. It is based on a laminar boundary layer and retains the conservation of energy. Despite the fact, that melting and evaporation have not been taken into account in the current modeling, test runs indicate that the temperatures observed in the real application can be matched.

This set up replicates conditions of a thermal spray gun to some extend. The real plasma arc is neglected, but all gas dynamic features are included. It would be the ideal tool for the development of guns for cold spray in the future.

2.3 Modeling of the Plasma Arc

In order to get closer to the real world of thermal spraying, the plasma arc has to be included. Additional physical models and the basic equations of electromagnetism have to be implemented and coupled to the commercial flow solver ANSYS CFX (Ref 3, 4) to form a magneto-hydrodynamic (MHD) model.

Radiation has to be treated as a temperature- and pressure-dependent net emission by an appropriate model (Ref 5-7). In order to get the arc started, some artificial, local heat sources are needed, which are switched off after the startup phase of the simulation. Sheath regions have, so far, been neglected, although they are present in the real application. Including them is possible, but does significantly increase the complexity of the simulations. They have been included for evaluation purposes, but a thorough analysis of the results revealed that neglecting the sheath regions basically results in a more or less systematic offset in voltage. Therefore the additional effort does not notably increase the information gained for gun design. The electromagnetism included consists of the Maxwell equations, material relations for polarization (permittivity), conductivity and magnetization (permeability). Coupling of electromagnetism and fluid dynamics is accomplished by Ohm's law, the Lorentz force and resistive heating, Fig. 1.

Within the fluid region the following equations are being solved for each iteration:

- conservation of mass (continuity equation);
- conservation of momentum (Navier-Stokes) with Lorentz force;
- turbulence model (standard *k*-epsilon model);
- transport equations for turbulent kinetic energy and dissipation;

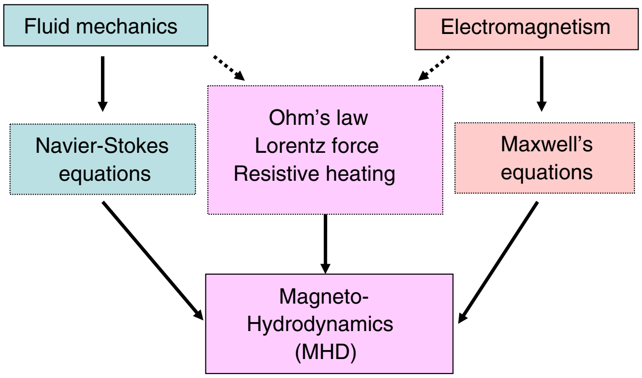

Fig. 1 Schematic of coupling between fluid dynamics and electromagnetism

- conservation of energy with resistive heating;
- charge conservation (Poisson equation for electric potential);
- magnetic vector potential.

Equations solved in the solid region around the nozzle concern the magnetic vector potential. In the real application the magnetic field is not restricted to the fluid region. In order to take this fact into account a region around the fluid domain in the area of the nozzle is discretized by a computational mesh, as well.

In order to solve this set of coupled equations for each cell of the computational domain iteratively the following numerical models are being applied:

- simulations are run in steady state, although it could well be that the real flow is transient at some locations. But running the simulations steady state, drastically reduces computer resources;
- single precision solver;
- full implicit second order discretization;
- same final residual target for all simulations in order to obtain results of the same accuracy.

The correct gas properties are very important for such simulations. For the time being, it is assumed that all values except radiation are in local thermal equilibrium. Therefore, properties like molar mass, viscosity, specific heat capacity, thermal and electrical conductivity, and sonic velocity are only temperature and pressure dependent.

Averaged measurements taken from a plasma gun running without powder can be directly compared to results of such simulations and are very important for the validation of this very complex setup.

2.4 Plasma Arc with Particles

The most complex, but most real model is the MHD approach outlined above with inclusion of the particle tracking. As mentioned before, standard particle tracking models are not intended for supersonic and plasma flows. In addition to the friction-heating model outlined before, correct drag and resistance prediction have to be tailored to these extreme-operating conditions. At these very high temperatures, up to 20,000 K, particles are melting and even evaporating, which calls for further modeling to include these features. Moreover spraying may take place with particles being made up of pure metals and therefore electromagnetic interaction of particles, like magnetization may be relevant. Modeling these physics is one challenge (Ref 8), but quantifying these phenomena by measurement techniques for validation purposes is even more demanding. Therefore, the application of a sophisticated 3D multi-instrument diagnostic system for the quantitative analysis of the particles/droplets exiting the nozzle is of high priority.

Running this complete simulation tool almost replicates the real world of plasma spraying. It can either be used to virtually test the entirely new or modified guns or to explore the feasibility of spraying new powders or operating under different conditions. However, until this task can be reliably accomplished more resources have to be spent for measurements and validation.

2.5 Typical Setup of a CFD Calculation

Figure 2 shows a schematic of the typical CFD procedure. The geometry being wetted by the fluid has to be modeled by a CAD system. Based on that model a computational grid is generated which divides the computational domain of interest into small elements. For each element the equations for fluid dynamics, and if activated, the equations for electromagnetism are solved. Meshes using hexahedral elements have been used for all simulations presented here. In order to reduce computing resources usually only a segment instead of the whole geometry is used for CFD applications. The geometry is completed in circumferential direction by the use of periodic boundary conditions. Figure 3 shows a typical arrangement of geometry and boundary conditions for spray gun simulations including MHD.

The next step is the actual computation of the case. Typical setups, as presented in this article, feature

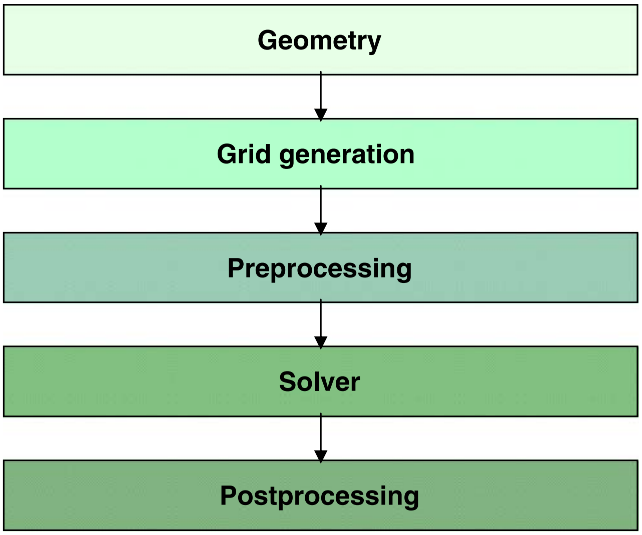

Fig. 2 Steps of typical CFD calculation

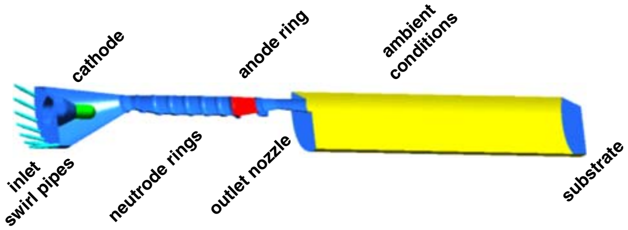

Fig. 3 Geometry and boundary conditions (one-third of actual geometry shown)

computational meshes of about one million hexahedras. Running the CFD code with MHD coupled on, e.g., eight processors on a Linux cluster results in a CPU time of about 24 h until converged results are obtained.

The postprocessing phase gives the actual insight into the flow and electromagnetic phenomena. Flow structures can be visualized by streamlines and vectors and contour plots provide information on scalar quantities in selected cross sections. Global performance data like, e.g., pressure ratios or losses can easily be computed from the CFD results.

3. Validation of Simulation Tools

Validation of such complex models is absolutely necessary. Although a single model may have been used for other applications, the combination of different models has to be tested. Moreover the limitations of the simulation tool have to be known in order to use it correctly. Further research into measuring techniques for particles melting or evaporating and traveling at high velocities is needed. In order to obtain good validation data special care is needed. The CFD engineer has to know exactly how the test rig is operated and how the measuring equipment is handled. The geometry of the test rig and the simulation model have to be absolutely identical. Fluid properties and operating conditions have to match, as well. In the CFD postprocessing the same quantities have to be processed at the same locations as in the measurements. Based on such test data, the numerical model can be calibrated, if necessary, and the influence of model parameters, boundary conditions, and computation meshes can be assessed.

4. First Experiences

For validation purposes and to assess the capabilities and limitations, as well as to gain experience, simulation tools have initially been used to analyze and optimize single parts of an existing spray gun. Selected examples are presented in the following paragraph.

4.1 Validation of the TriplexPro^{TM}-200 Plasma Gun

First MHD simulations have been run for the TriplexPro^{TM}-200 plasma gun of Sulzer Metco, Fig. 4 (the setup and boundary conditions are presented in Fig. 3). Preliminary tests revealed the necessity of including the Lorentz force in the model. If not included, three separate arcs stretch from the cathodes to the anodes. Activating this force in the model leads to a unification of the three arcs downstream of the cathodes (Fig. 5) and the velocity field gets more homogeneous at the nozzle exit (Fig. 6).

In a plasma-spray gun the fluid moving in an external electric field is causing a current density which comprises of three electric arcs and in turn causes an electric field. The interaction of the magnetic field with the current density causes the Lorentz force, which acts on the three arcs. The current is aligned along the main axis (Fig. 7), and the magnetic field is oriented clockwise concentrically around the current, therefore the resulting Lorentz force points inwards (Fig. 8).

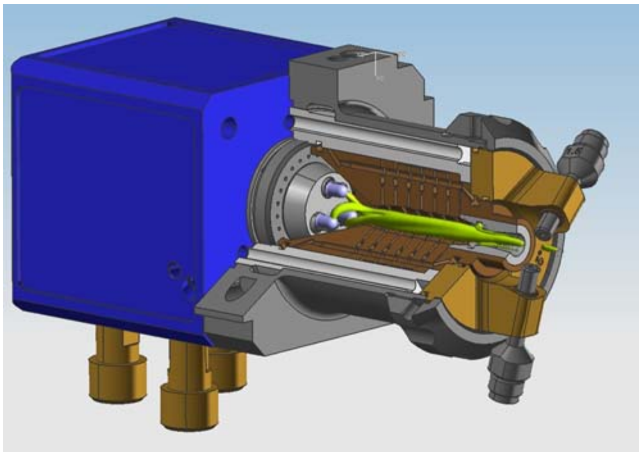

Fig. 4 Sulzer Metco TriplexPro^{TM}-200: CAD and simulated plasma arcs

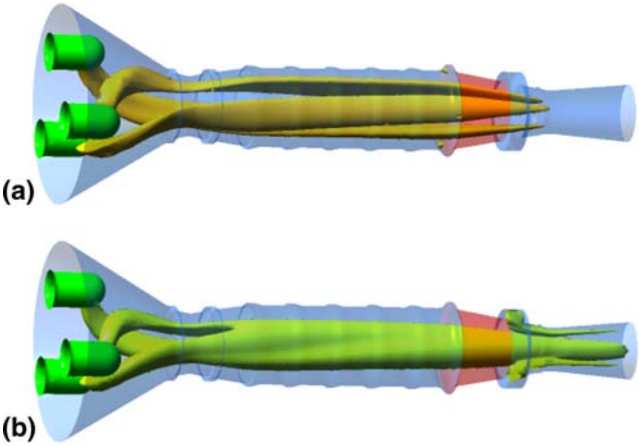

Fig. 5 Iso-surfaces of temperature represent hottest areas for plasma arc without (a) and with (b) Lorentz force

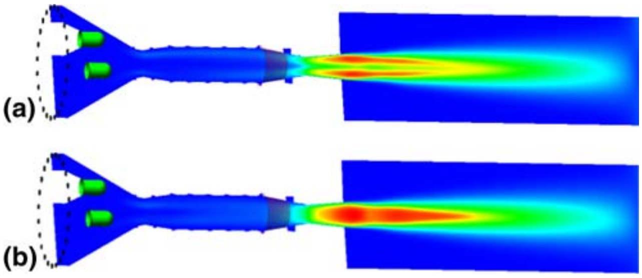

Fig. 6 Velocity distribution of gas flow for plasma arc without (a) and with (b) Lorentz force (red = high, blue = low velocity magnitude)

Fig. 7 Visualization of current density (red = high, green = low) in-between the three cathodes and the anode ring with Lorentz force

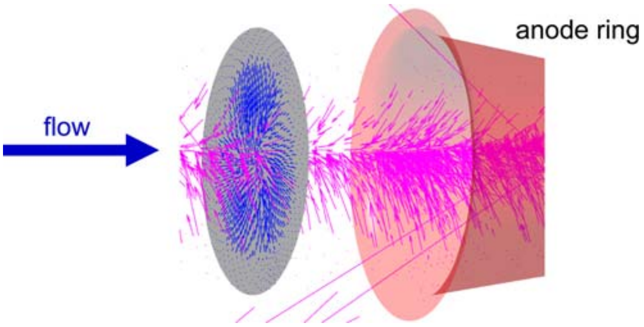

Fig. 8 Lorentz force represented by vectors in the region of the anode ring

This test clearly illustrates the necessity of direct coupling between fluid dynamics and electromagnetism. If the physics of electromagnetism is only calculated within the postprocessing of a gas-only simulation, the same gas flow field would be present whether the Lorentz force is activated or not. For validation purposes, several sets of operating conditions have been run. The geometry has been kept unchanged while the gases, gas flow rates, and electric currents have been changed within a realistic range. Table 1 shows the operating conditions used for the first validation. The properties of the gas mixture Argon-Helium are computed within the code according to the following rules: the density is volume fraction weighted, while viscosity, thermal conductivity, and specific heat capacity are mass fraction weighted. Mass fraction weighting is used for the calculation of electric conductivity.

In the simulation, the operating condition is set by the flow rate and electric current. Gas pressure and potential are then a result of the calculation and can be compared to the test data. First validation results are listed in Table 2.

Table 1 Operating conditions used for validation of MHD tool

Case	Gas	Flow rate, SLPM	Inlet temp., °C	Ambient pressure, Pa	Current, A
1	Ar	140	20	100,000	360
2	Ar	140	20	100,000	450
3	Ar	140	20	100,000	500
4	Ar/He	90/50	20	100,000	360
5	Ar/He	90/100	20	100,000	360

Table 2 Comparison of computed voltage vs. experimental voltage

Case	Gas	Current, A	Experimental voltage, V	Commutated voltage, V	Experimental-computed, %
1	Ar	360	118.9	139.0	16.9
2	Ar	450	126.0	137.7	9.3
3	Ar	500	129.5	140.1	8.2
4	Ar/He	360	120.2	133.2	10.8
5	Ar/He	360	133.0	136.3	2.5

With the exception of case 1 all other predictions of voltage by MHD are within 10% of the average values measured during testing. These results are quite remarkable as they have been obtained by a simulation setup which has been run as a complete set for the first time without any parameter tuning based on experiments. The fact that voltage prediction is in general too high suggests some systematic offset that could be verified and, if necessary, corrected by further validations. Observations of wear traces in a spray gun which has been operated for some time can be used for qualitative validations. For example, the emission points of the arcs on the electrodes leave marks on the surface due to the extreme temperatures. This can be directly compared to MHD results by plotting an iso-surface of temperature to visualize the arcs as shown in Fig. 9. The comparison illustrates that the location of the arc emission can be quite well captured by the simulation.

In Fig. 10, bottom, a view in streamwise direction into the chamber of the spray gun is shown. This chamber has been in use during testing and shows some wear that can be used for qualitative CFD validation. Dark traces around the periphery (one is marked by an arrow) show the direction of the individual gas jets entering the chamber. The swirl is induced by the orientation of the tubes. Further downstream a dark circle is visible, in Fig. 10 highlighted by a black circle. This is the consolidation point, where the individual gas jets merge into a single-swirl flow. This nicely corresponds with the location of the consolidation point in the computer model about two-third the way down the chamber, Fig. 10, top. The three distinctive dark patches are where the arcs first strike during ignition.

Validation work is going on to further strengthen the confidence in this very powerful simulation tool.

5. Advantages of Simulation Tools in the Spray Gun Design

Before the introduction of CFD spray gun development has been strongly based on experience and experiments and to some extend on trial and error. The use of simulation tools gives for the first time a detailed insight into various physical phenomena previously not accessible. Many of them have up to now not well been understood. Careful analysis and postprocessing can reveal areas with potential for improvement.

The use of validated simulation tools considerably reduces the need for prototype manufacturing and experimental studies. This in turn reduces time to market

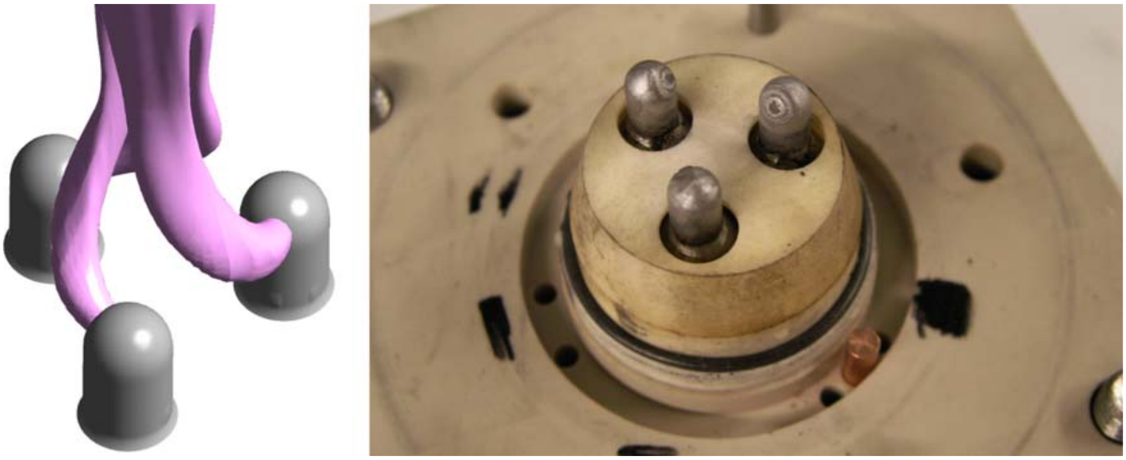

Fig. 9 Left, predicted emission points at cathodes (insulator removed for clarity) and right, TriplexPro^{TM}-200 cathodes and insulator after testing

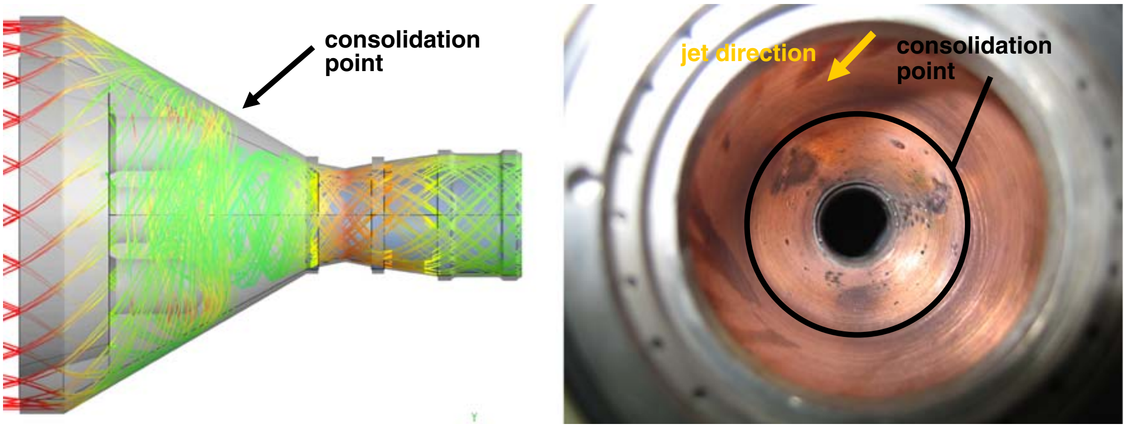

Fig. 10 Left, predicted streamlines of gas flow in chamber and right, TriplexPro^{TM}-200 chamber showing traces of gas flow

of a new or modified product and leads to more advanced and optimized spray guns. Furthermore new operating regimes and areas of application can be explored without any physical risk. First applications of simulation techniques to spray-gun development at Sulzer Metco proved these statements and further integration into the design process is therefore of high priority.

6. Conclusions

Numerical models have been introduced into the design and modification process of spray guns. Starting from standard CFD applications the modeling has been extended to include particles and the plasma arcs. The latter ones called for a rather complex coupling of the electromagnetism to the fluid dynamics. Extensive testing and validation revealed the accuracy and limitations of the simulation tool. First applications show the feasibility of improving spray guns based on simulation results. The rear chamber of the Sulzer Metco TriplexPro^{TM}-200 could be freed from excessive heating of the insulator. Using a full magneto hydrodynamic model for the same gun will lead to an optimized spray process and hence better economics. The need of a direct coupling between fluid dynamics and electromagnetism could be nicely illustrated by running the MHD tool with and without Lorentz force. By activating the Lorentz force the three separate arcs are unified and by interaction alter the flow pattern of the gas flow. By running MHD in the postprocessing of a CFD code, such real world interactions could not be predicted. Further applications of these computer models are thoroughly covered in a companion paper to this presented in this volume (Ref 2).

Integrating the CFD and MHD codes into optimization software could lead to an automatic optimization of certain parts of a spray gun in the future. The designer has to define a set of target values which are ideal for the specific application and then the code, by use of optimization algorithms, does automatically compute various scenarios until converging on an optimum configuration, e.g., an optimized outlet nozzle. A further opportunity to use these simulations tools is the exploration of new operating regimes which currently cannot be supported by the physical hardware.

The use of CFD in solving problems provides an economical alternative to physical prototyping on a trial and error basis and brings additional understanding as to the nature of flow related problems.

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