

Complete design of a high power ultrasonic flow-cell reactor with special air cooling system

L.Spicci,

Everywave Srl, Via dell'Artigianato 27/28, 35010, Villa del Conte (PD), Italy

Introduction

Ultrasonic flow-cell reactors are used for many industrial applications, where fluid substrate is sonicated in a small region, where very high ultrasonic acoustic power is present. The electromechanical transducer ("converter") that drive the sonotrode inside the flow-cell is designed with Comsol Structural mechanics, Acoustics and SolidWorks livelink module, to get a reliable, efficient and flexible design, thanks to special tuned metal parts and high efficiency hard PZT piezoelectric ceramic rings. Efficiency of such device can reach up to 98%, so thermal loss are quite low. Such results were possible making use of a novel converter structure, that employs two stacks of piezo-rings, with proper positioning in nodal points and phasing. Nevertheless, since the reactor may be in service 24 / 7 and piezo material cannot operate above 150°C, thermal management solutions are very important. Among these, best would be to employ a liquid cooling system inside the converter, where heat is generated, but the device is not generally compatible with standard liquids and the solution could be quite complicated. On the other hand, a high pressure / low flow cooling air (used as standard with such type of devices) cannot guarantee a proper cooling at 3kW power level or more. So a novel low pressure / high flow system was conceived for the application, making use of Comsol Fluid-flow and Heat-transfer modules, in order to get an efficient thermal drain and temperature control.

High power Ultrasound and Cavitation

Sonochemistry and ultrasonic processing of fluid products are based on the phenomenon of cavitation. While cavitation is the most well-known phenomenon linked to the passage of ultrasound through a liquid medium, it is also perhaps the least understood [1]. Cavitation in a liquid occurs due to the stresses induced in the liquid by the passage of a sound wave; in fact the sound waves consist of compression and decompression: if pressure gets sufficiently low, the liquid can be torn to pieces to leave small bubbles. These cavitation bubbles (similar to those seen from the action of a propeller of a boat on water) are the heart of the sonochemistry systems. Being subject to the stresses induced by sound waves, the bubbles grow

during a decompression phase and contract or even implode during a compression phase. The bubbles can be filled with steam and gas and can produce radicals during implosions. It is these implosions that are the high-energy part of sonochemistry: each of these imploded bubbles can be seen as a micro-reactor, with actual temperatures reaching an estimated 5000 ° K and pressures of several hundred atmospheres [2],[3]. When bubbles collapse, powerful shock waves occur.

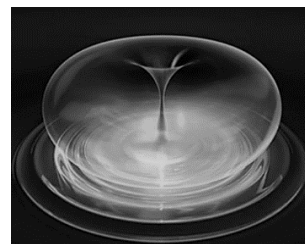


Figure 1: cavitation

These shocks are believed to be responsible for breaking nearby solids and also lead to the generation of shear forces and vortices [1] which in turn can lead to an increase in turbulent energy dissipation.

In industrial applications such as deagglomeration, dispersion, homogenization, emulsion, the strength of ultrasonic mixing can be explained as a special phenomenon of turbulence, due to the shock waves generated by the implosion of cavitation bubbles, which can lead to large increases in the mass transfer coefficient with respect to traditional mixing systems. Of course shock waves originated from cavitation are related to the intensity and frequency of the ultrasonic wave.

Cavitation is classified mainly as two types, transient and stable. The type of cavitation that occurs mainly depends on the energy introduced: at higher intensities (10W/cm²), transient cavitation predominates, while at lower energy levels (1-3W/cm²) stable cavitation takes place.

Finally, cavitation bubbles are dependent on ultrasonic frequency: low frequency ultrasounds (20-30kHz) produce larger bubbles and violent cavitation, leading to higher temperatures and pressures. Instead high frequency ultrasounds (40-80kHz) result in a less violent cavitation effect but more cavitation events may occur.

Ultrasonic High-power, Flow-cell Reactor

The 3D model of the ultrasonic system is reported in figure 2 (with and without flow-cell, to see the sonotrode inside).

The system consists of three parts:

- 20kHz piezoelectric transducer or 'converter'
- 'Booster'
- Sonotrode with 'tuned rings', named 'steprod'
- Cylindrical reactor or 'flow-cell'

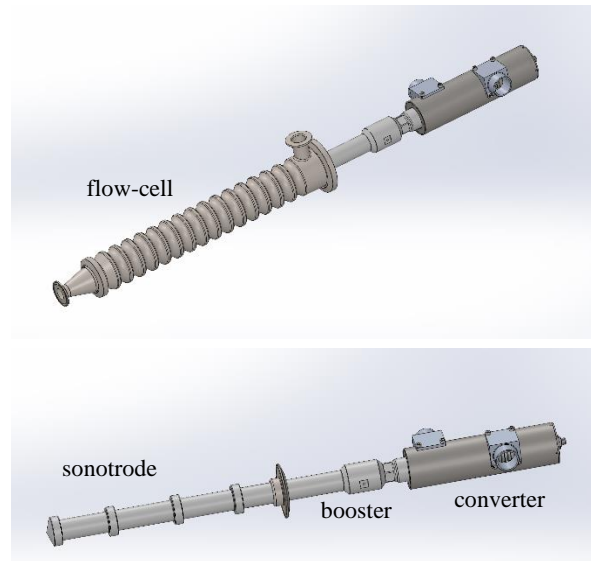


Figure 2: ultrasonic reactor (with / without flow-cell)

The electromechanical transducer or 'converter' is based on a novel conception of the standard 'Langevin structure', with many design details and innovations to get the maximum efficiency.

Just to name one, the present converter is not based on a single stack of Hard-PZT piezoelectric rings (as usual), but on two stacks. In fact the total power of an ultrasonic converter is usually dependent on the total volume of piezo-ceramic employed.

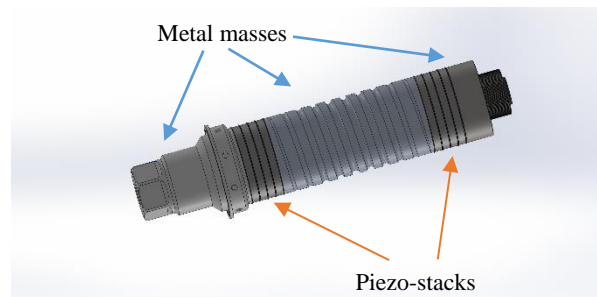


Figure 3: ultrasonic converter (without cover)

Therefore such design can be used to get a more powerful system, but maximum and minimum vibration regions must be analyzed. These latter are named nodal region, where piezo-stacks should be placed to get maximum efficiency and minimum stress. Of course FEM is the best tool to build such structure, performing an optimization process of the piezo-stack positioning.

Moreover, both piezo-stacks should be pre-stressed through a central bolt at very high pressures, thus requiring a special tensioning device.

As regard polarization and driving voltage of the piezo-rings, connections are performed so that the two piezo-stacks operate electrically parallel, mechanically series but with opposite displacement, so that the central mass 'floats' and results in a large vibration amplitude on the front mass, that is connected to the sonotrode.

The booster is a standard device that 'boosts' the amplitude of vibration on the thinner side with respect to the thicker one (with nodal region in the middle), as can be easily understood. Such device is important to limit the required electrical current to drive the sonotrode vibration and reduce the piezo-rings fatigue, thus resulting in a higher possible operating power.

As regard the special sonotrode with 'stepped tuned' rings named 'steprod', it is a very complicated part to design because the geometry of the rings on the rod must be studied carefully to guarantee a high level of pressure field in the surrounding fluid and, on the other hand, to limit spurious resonances close to the main one, which may be generated by the complex geometry.

Also the geometry of the surrounding cylindrical flow-cell reactor is important for the optimization of the main resonance and for the homogeneity of the pressure field in the fluid.

Indeed the shape of the reactor was deeply analyzed through FEM and special features were developed to reduce the transmission of undesired vibration along the flow-cell walls: it's clear from first part of figure 2 that a special 'wave-crest' external surface shape was optimized to act as a suspension that dampens the undesired vibrations.

The electro-mechanical system is thus critical to design and optimize, in order to yield very high acoustic power densities, as required for the industrial applications. If a deep modeling and optimization procedure is performed, the final result is a very efficient system that dissipates a very low amount of energy.

Nevertheless, since the reactor may be in service 24 / 7 and piezo material cannot operate above 150°C, thermal management solutions are very important.

The dissipated thermal power must be drained from inside the converter, in order to keep the piezo-ring temperature constant and well below 150°C.

Of course the most effective type of cooling would be a liquid-based system, but a generic fluid is critical to get in contact with piezo-ceramics, since these are connected to very high driving voltage and possible cavitation effects are to be avoided on the piezo-rings external vibrating surface. On the other hand a typical high pressure / low flow cooling air (used as standard with such type of converters, flowing through small connectors on the cover back) cannot guarantee a proper cooling at 3kW power level or more.

So a novel low pressure / high flow system was conceived for the application, making use of Comsol Fluid-flow and Heat-transfer modules, in order to get efficient thermal drain and temperature control. Basically such solution is based on an external impeller that forces high flow of air into quite large input port on the converter cover, placed so that the air flow wraps around the central mass of the converter end exits tangentially from the exit port, resulting in an efficient heat drain.

Model description

A detailed FEM for the ultrasonic reactor was built using COMSOL Multiphysics® 6.1, making use of Solid Mechanics, Piezoelectric, Acoustics, Fluid flow and Heat transfer modules.

First a brief description of the Structural & Piezoelectric model is reported.

Axial symmetry couldn't be exploited to reduce model dimensions since the fluid cell and cover are not axial-symmetric. So symmetry was used to cut the model in half on a 3D model. Mesh on all domains was chosen as free tetrahedral and element size was always less than a fifth of signal wavelength.

As already mentioned, the electro-mechanical converter is based on two prestressed stacks of four hard-PZT-8 piezoelectric rings each, that work electrically parallel, mechanically series but the two stacks oscillates with opposite phase. That is, when one stack expand, the other compress in such way that the middle metal mass 'floats' and control the front vibration through the central hub. That design is very efficient in terms of maximum front vibration amplitude and minimum piezo-ring stress, along with minimum back vibration.

As regard piezo material, hard PZT-8 type ceramic is chosen as active medium, due to its exceptionally high efficiency and Q factor.

The 3D drawing of such transducer is reported in figure 3 and vibration maps will be reported in the following.

It's to be noted that the design of the three metal parts that enclose the piezo-stacks are critical, since they are responsible for: tuning, efficiency and vibration amplitude of operation.

With a standard Langevin structure, with only one stack of piezo-rings, they are generally called 'backmass' and 'frontmass', but in the present design we have also a large 'middlemass', between the two piezo-stacks.

Backmass (where the bolt tension the internal hub) is made of steel, middle-mass is made of Aluminum and the front-mass is made of Titanium alloy (grade 5). The frontmass must also include a mechanical suspension system, in order to decouple radial undesired vibration modes from the cover.

In the present work, the converter was designed to operate with a resonance frequency of 20kHz with operating power up to 3kW.

As regard piezoelectricity, the constitutive equations for the material are [4], in *stress-charge* form :

$$\begin{cases} \mathbf{T} = [\mathbf{c}^E] \mathbf{S} - [\mathbf{e}'^T] \mathbf{E} \\ \mathbf{D} = [\mathbf{e}] \mathbf{S} + [\boldsymbol{\epsilon}^S] \mathbf{E} \end{cases} \quad \text{Eq.1}$$

where \mathbf{T} is the stress vector, \mathbf{c} is the elasticity matrix, \mathbf{S} is the strain vector, \mathbf{e} is the piezoelectric matrix, \mathbf{E} is the electric field vector, \mathbf{D} is the electric displacement vector, $\boldsymbol{\epsilon}$ is the dielectric permittivity matrix. The superscripts indicates a zero or constant corresponding field. Eq.(1) takes into account both piezoelectricity, both mechanical and electrical anisotropy of the material.

Once these matrices have been specified, COMSOL recognizes which equations domains are to be used inside the FEM elements.

Piezoelectric Material and Electrostatics were imposed on the eight piezoceramic rings inside the transducer, were ground and electric potential were set alternately to get electrical parallel connection. Polarization directions of the piezomaterials were selected to get the opposite phase oscillation of the two stacks reported before.

Next the booster and special sonotrode were designed and optimized.

Booster must be designed to match the operating resonance frequency (its length must be approximately half wavelength) and amplify vibration amplitude on the lower radius side.

As regard the sonotrode, the ‘tuned rings’ are needed to increase the coupling surface and get stronger cavitation in the surrounding fluid, but need to be designed carefully, along with the sonotrode total length, to perfectly match the converter and booster resonance frequency.

Another important element is the flange that connect the sonotrode to the reactor, as that element has an integrated mechanical suspension to decouple radial vibration from the reactor.

The cylindrical flow-cell reactor was designed, so that the acoustic domain could be delimited between reactor and sonotrode.

Acoustic-structure interaction is automatically set on the steprod and reactor corresponding surfaces.

In the Acoustic module it is possible to study the pressure field generated by the steprod, to check for the required pressure level, required to get strong cavitation for industrial applications.

Finally, as anticipated, the final and very important step of FEM simulation was the design of a novel thermal managing solution, to control the operating temperature of the converter. That was performed adding Fluid-flow and Heat-transfer physics to the ultrasonic converter model, in order to analyze cooling air flow and efficiency of the impeller-based solution. Such modules work together to model a nonisothermal flow with conjugate heat transfer and allows to calculate the temperature of piezo-rings inside the converter, that acts also as heat sources.

While the pressure and the velocity fields are the solution of the Navier-Stokes equations in the Fluid-flow module, the temperature is solved through the heat equation in the Heat transfer module. All these variables are related through multiphysics couplings.

Finally the mesh of the model is reported to complete the present description (for the structural simulation, ¼ section).

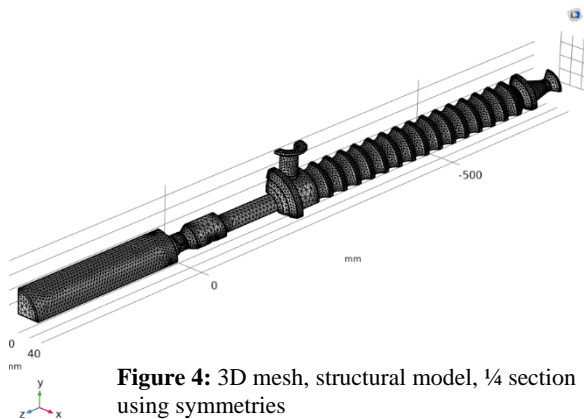


Figure 4: 3D mesh, structural model, ¼ section using symmetries

Simulation Results

The most important results of simulations are reported here.

The following data are the result of the complete design and optimization process, which is not described for the sake of brevity.

Mechanics

First the frequency analysis for the mechanical vibration of converter+sonotrode assembly (and with flow-cell filled with water as fluid medium) is reported, so that the main resonance frequency is defined.

Driving power is approx.3kW for the following results.

As it's clear from the electrical impedance plot below, a strong resonance is present at 20.05 kHz, as required, and the electrical impedance at resonance is approx. 80Ω.

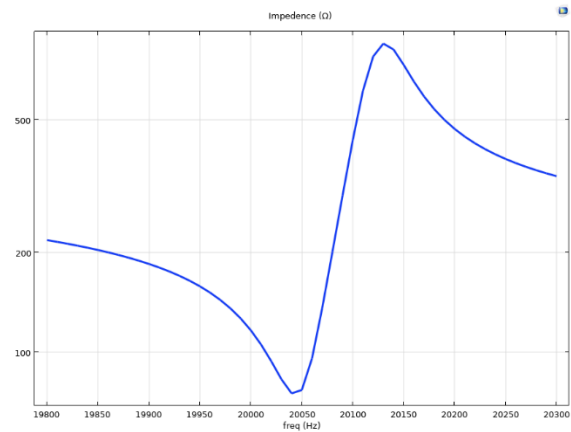


Figure 5: Electrical Impedance

Next, on the vibration vs. frequency plot two points are reported: the end of sonotrode and the side of connection flange to flow cell. The first vibrates with amplitude up to 24μm while the latter vibrates only with 1.5μm amplitude. That is a good result, as it's important that vibration is not wasted on transverse undesired directions and overall efficiency is high.

Moreover, a vibration map of the entire structural domain is reported, at resonance frequency: again, it's clear that the sonotrode vibrates with amplitude much higher than the flow-cell, as desired.

It's important to note that the ‘wave-crest’ external shape of the flow-cell is the result of an optimization process to reduce its undesired vibration, that was not acceptable with standard pipe-like flat shape.

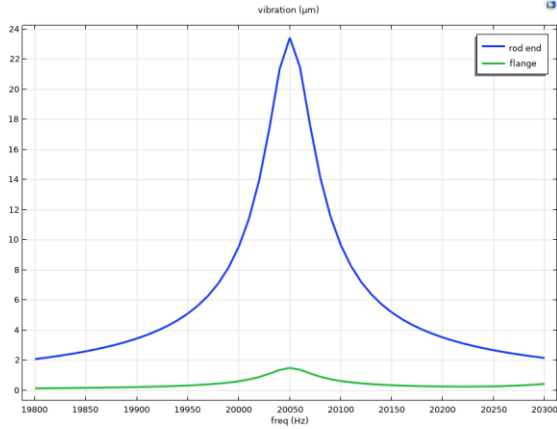


Figure 6: vibration amplitude

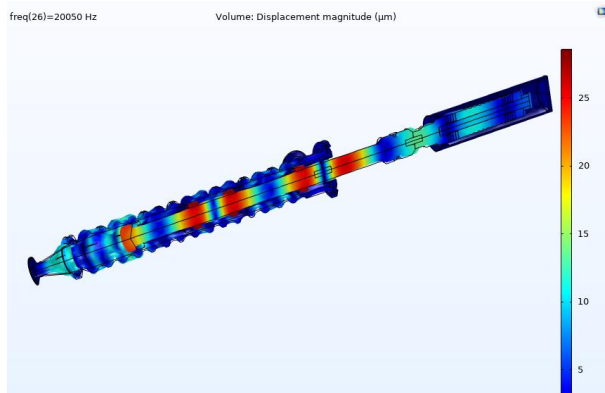


Figure 7: vibration 3D map

Acoustics

In the acoustic domain it's possible to check the pressure map in the fluid, at resonance frequency, as follows :

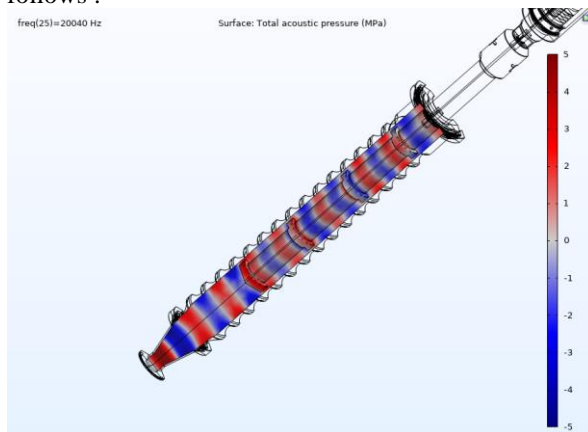


Figure 8: Pressure field

5MPa of ultrasonic pressure amplitude are available at 20kHz (with max values close to the rings), which is enough to get very strong cavitation phenomena in the fluid, as required for industrial applications.

Thermal Analysis

Finally, as anticipated, Fluid-flow and Heat-transfer physics were added to the ultrasonic converter model, in order to analyze cooling air flow and efficiency of a novel impeller-based solution.

The final cooling system geometry is the result of an optimization process which is not described for the sake of brevity.

The novel high flow / low pressure solution (from an impeller) is compared to the typical high pressure / low flow standard system (compressed air flowing through small connectors on the cover back) in order to assess the cooling improvement.

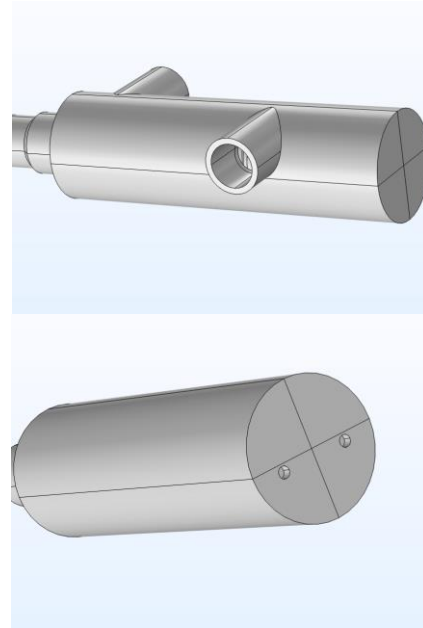


Figure 9: simplified models of new /old cooling systems

Fluid flow, air speed and temperature maps are reported for the standard and novel cooling systems. Typical values for air speed and pressure were used, accordingly to the type of system.

As regard heating caused by losses, a heat source was considered in the piezo-ring volume, corresponding to 30W (2% losses at 1.5kW operating power).

Next results clearly show a large improvement with the novel impeller based system, that leads to a omogeneous air flow, entering from the input port,

spinning around the central mass of the converter and exiting from the out port. With the old configuration there's no effective air movement inside the converter, leading to a much higher operating temperature.

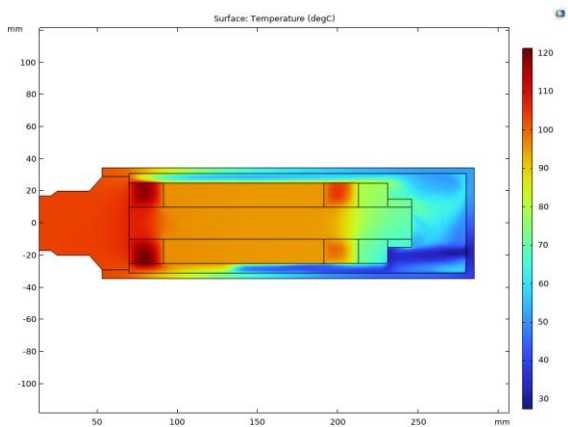
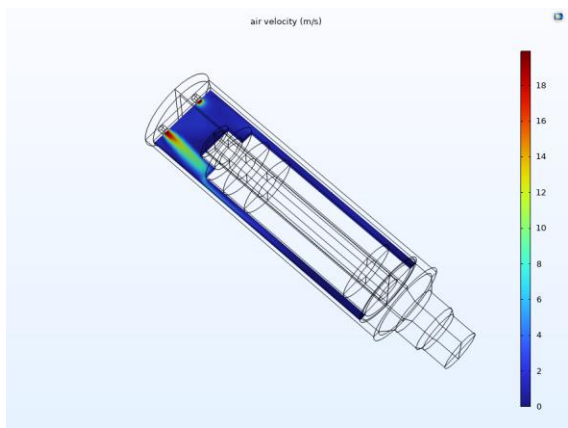
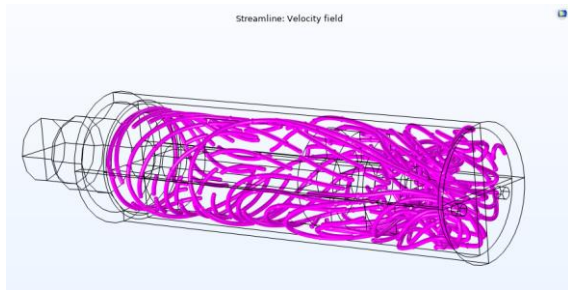


Figure 10: thermal results with old cooling systems

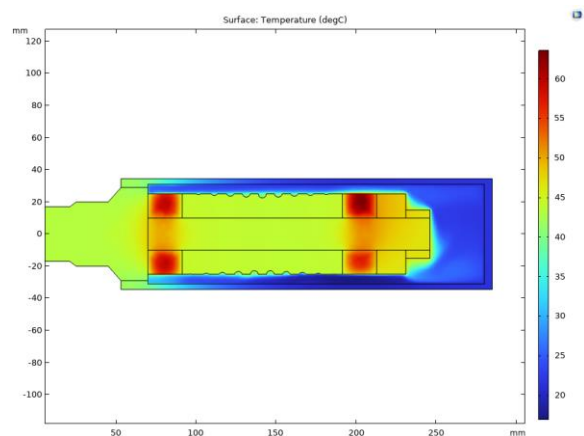
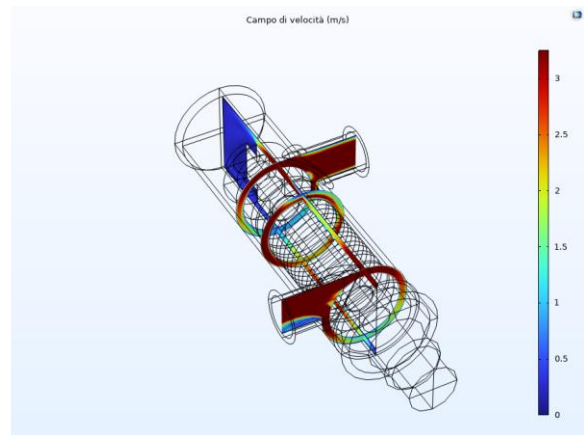
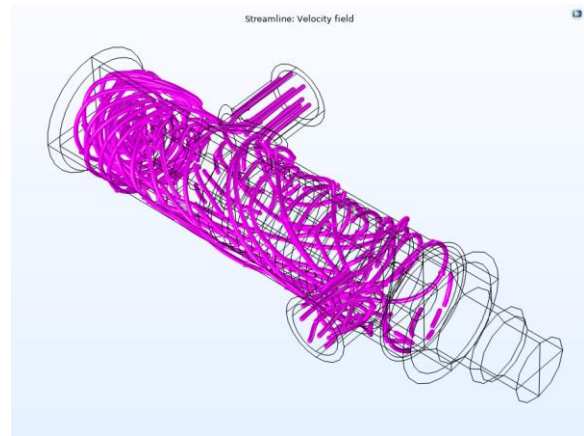


Figure 11: thermal results with novel cooling systems

From the temperature maps, at 1.5kW operating power the novel cooling system leads to 60°C maximum temperature for the piezo-rings, to compare with 120°C obtainable from the old system.

Conclusions

COMSOL Multiphysics® was used to design a multi-purpose ultrasonic reactor, consisting in a high-power piezoelectric converter, a cylindrical flow cell and a special sonotrode.

The design involves a special converter structure, that employs two stacks of piezo-rings, and a novel cooling system, based on an external impeller that forces high flow of air into quite large input port on the converter cover, so that the air flow wraps around the central mass of the converter end exits tangentially from the exit port, resulting in efficient heat drain.

The system was designed with a parametrized structural / acoustic / heat transfer & fluid flow multiphysic model and a complete optimization process was performed.

The simulation results were up to the required level of efficiency and very high levels of cavitation could be obtained in the reactor, in order to fulfill new industrial demands.

Moreover, the novel cooling system reduces the piezo-rings operating temperature value to about half compared to the old one, allowing for a higher level of continuous operating power.

References

1. Mason, T.J. & Lorimer, J.P. (2002), *Applied sonochemistry: The uses of power ultrasound in chemistry and processing*, Wiley-VCH
2. Mason, T.J. (1997). *Ultrasound in synthetic organic chemistry*, Chemical Society Reviews, 26, 448.
3. Thompson, L.H. & Doraiswamy, L.K. (1999), *Sonochemistry: Science and engineering. Industrial & Engineering Chemistry Research*, 38(4), 1215-1249
4. COMSOL Multiphysics Module User Guide