Numerical Modelling and Performance Optimization Study of a Diaphragm Pump for Drug Infusion

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Abstract: In this contribution we present the results of the numerical modelling and performance optimization study of a diaphragm pump for drug infusion. The main objective is to develop a numerical model that replicates the pumping cycle (400ms) and also provides indications about the variation of pumping performance as consequence of the variation of the chamber-diaphragm system geometry, diaphragm materials and other operating conditions (backpressure and working fluid). In the first part a brief description of the pump, computational domain, boundary conditions and governing equations of the model will be presented. The structural behaviour of the diaphragm subjected to the forces of the electromagnetic actuation system will be showed. In particular the effect of the different diaphragm material and the stress state with different geometry will be analyzed. The fluid dynamic effect of the diaphragm movement will be transferred to the fluid inside the pumping chamber and then at intake-exhaust system. The results of the numerical simulations will be showed in order to identify the relevant geometrical parameters and select the best solution in order to improve of the pumping performance.

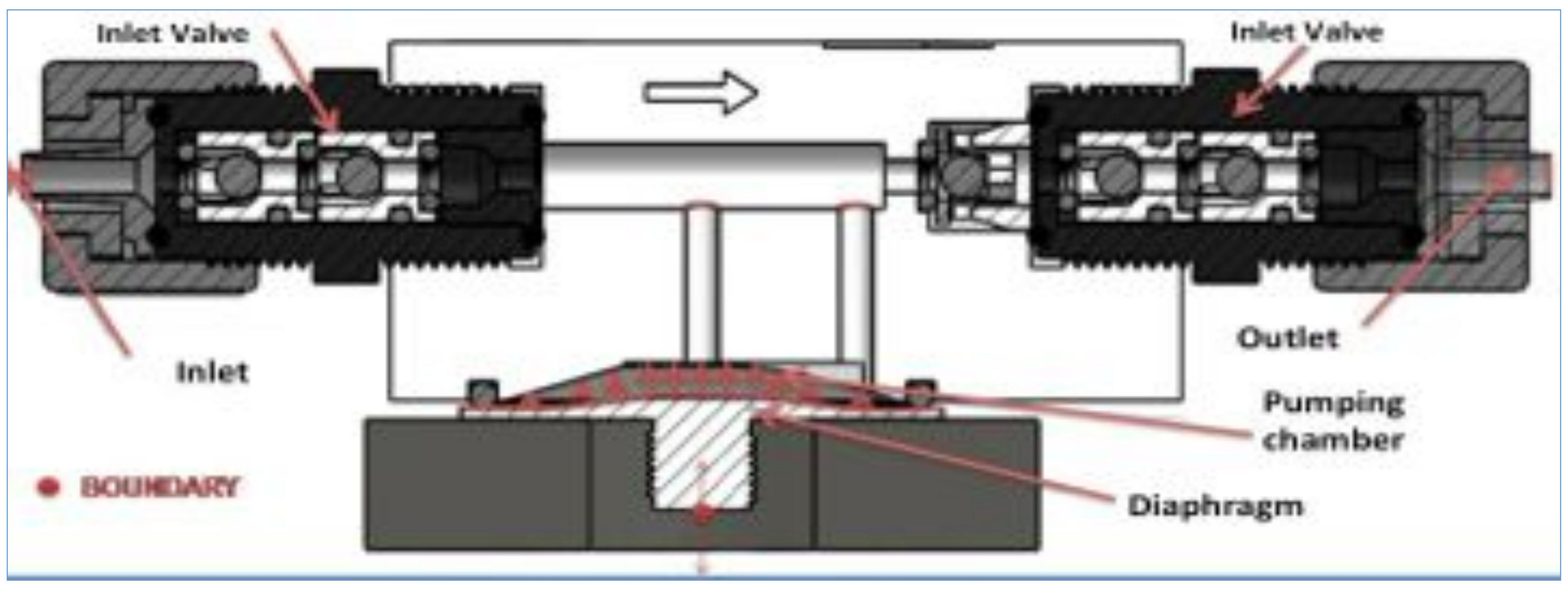

Figure 1. The diaphragm pump geometry (not to scale). Inlet/outlet valves (in red), pumping chamber and diaphragm are represented

The pump characteristic and working principle : The diaphragm pump, the object of the study, uses a combination of the reciprocating action of a polytetrafluoroethylene (PTFE) diaphragm, actuated by an electromagnetic system, and spherical valves. In this contribution, for simplicity, the electromagnetic system has not been modelled. The optimal pump design depends on the application, and most specifically on the elastic properties and geometry of the diaphragm and the characteristic of the working fluid. The pump flow rate is proportional to the number of strokes of the electromagnetic system for each single injection. The geometry of the pump was supplied by constructor and is illustrated in Figure 1.

Computational domain and boundary conditions: Based of the geometrical and operative details provided by the constructor (Figure 1), the 3D structural and fluid domain of the pump has been reproduced. The mesh, represented in Figure 2, is composed of about 84000 tetrahedral elements. Constant pressure boundary conditions are imposed for inlet and outlet of the fluid domain and an external force has been applied to the diaphragm stem in order to reproduce the effect of the electromagnetic actuator according with the measurements performed by the constructor.

Governing equation: Due to the complexity of the device, results are obtained stepwise, performing preliminary analyses with simplified models and then by gradually coupling the models introducing the different physics involved. The pumping process is a fluid-structure interaction problem with strong coupling between the solid and fluid domains. The continuum hypothesis for fluid modelling is still valid at the size scales of these devices. The fluid flow is described by the Navier- Stokes equations with turbulent (RANS standard k-ε model) incompressible, homogeneous and Newtonian flow. The working fluid is assumed to be water (density ρ_w = 1000 Kg/m^3 viscosity μ_w = 0.001 Pa·s) @298.15K. The model can take into account the effect of the variation of thermo-physical and viscous quantities of the fluid due to the changing of the operative temperature. The model also can easily be modified to manage fluid with high viscosity or non-Newtonian fluid. The model has been used to valuate the pumping performance with different characteristics (density ρw = 1098 Kg/m^3 viscosity μ_w = 0.1 Pa·s) of the fluid. The deformation of the diaphragm has been modelled by using COMSOL Structural Mechanics Model. The diaphragm is made of PTFE, modelled as isotropic linear elastic (Young's modulus E = 365 MPa, Poisson's ratio υ = 0.46, density ρ = 2150 Kg/m^3). The diaphragm elastic behaviour has been assessed also by using a different material, polyvinylidene fluoride (PVDF) (Young's modulus E = 200 MPa, Poisson's ratio υ = 0.34, density ρ = 1780 Kg/m^3). Large deformation formulation has been included in the model. A non-slip FSI boundary has been set up. The fluid structure interaction has been simulated by using an Arbitrary Lagrangian-Eulerian (ALE) formulation. This involves a Lagrangian framework for the solid and an Eulerian framework for the fluid. A moving mesh model has been used to take into account the deformation of the diaphragm and the effect of this deformation on the fluid. Time-dependent solution is obtained by an implicit solver (backward Euler integration).

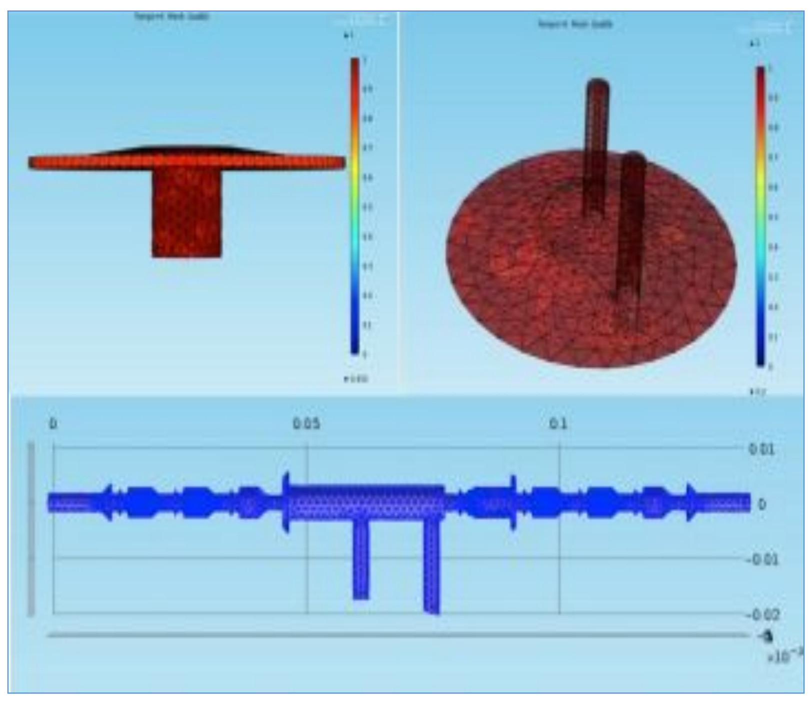

Figure 2. Computational domain: Diaphragm (top left) pumping chamber (top right) and valves (bottom) .

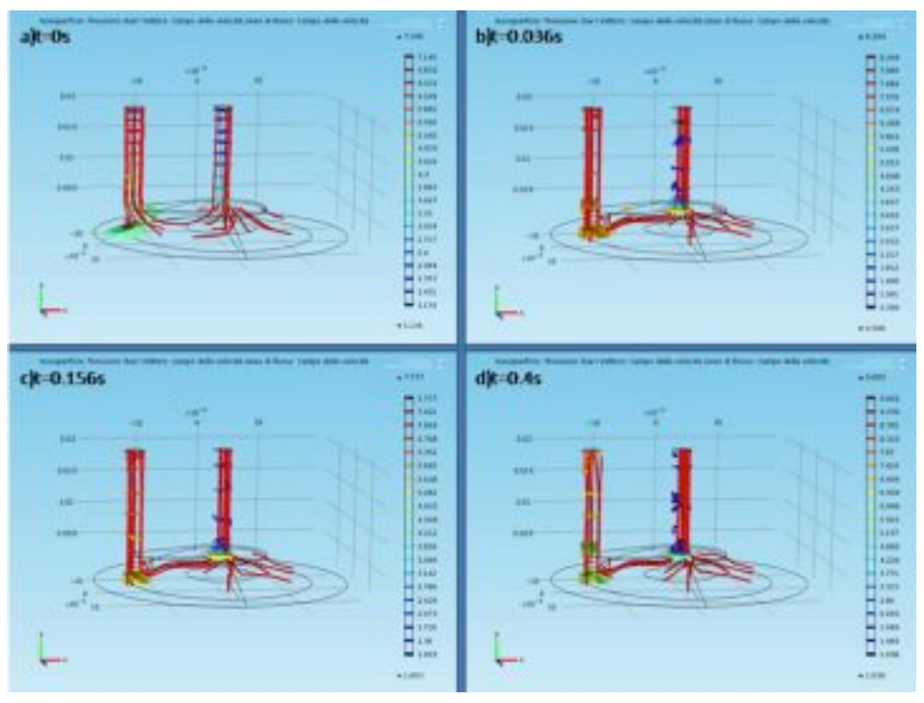

Figure 3. Pressure and velocity field inside the pumping chamber ford the standard molded geometry during the pumping cycle (0s-0.036s-0.156s-0.4s).

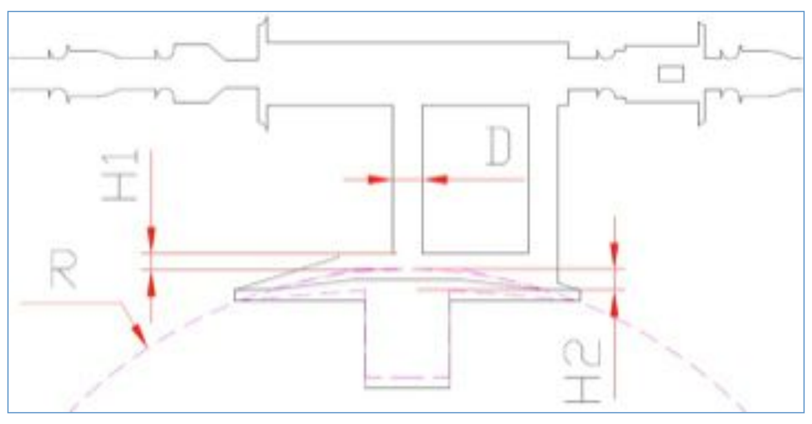

Figure 4: Relevant dimensional parameter for the geometrical optimization.

4. References

1. E. Becker, **Mechanically Driven Diaphragm Pumps for Use with Gases: Fundamentals - design – applications**, Vulkan Publishers (1997)

2. COMSOL Documentation**: Structural Mechanics Module**, COMSOL 4.2 (2011)

3. F.M. White, **Viscous Fluid Flow**, section 3- 3.3, McGraw-Hill, New York (1991)

Results: The numerical characteristic curves of the pump have been obtained by imposing the boundary conditions for the different operative conditions (backpressure and pumping frequencies), provided by the constructor. The diaphragm oscillations generated at the dead centers showed an amplitude about of 0.5/10 mm and were considered during the geometric optimization (reduction of dead volume). These oscillations were considered also to avoid possible interference between the diaphragm and the pumping chamber. The pressure and velocity field inside the pumping chamber for the standard molded geometry, are shown in Figure 3. In this paragraph results have been obtained with different diaphragm geometries: the present molded configuration, the configuration with a totally flat diaphragm, and an optimized molded configuration (molded-upgrade). The molded-upgrade diaphragm has been designed (see Figure 4) in order to minimize at top dead center the distance (H1) between the top of the pumping chamber and diaphragm and (H2) between the top diaphragm and the points where the diaphragm is sealed to the pumping chamber. The radius of curvature (R) of the diaphragm has been changed in order to obtain a spherical configuration at the top dead center. In such deformation condition the dead volume can be minimized and the stress distribution can be more regular.

Effect of different diaphragm materials: The choice of the material does not substantially affect the diaphragm active area, i.e the zone were the deformation is useful for the pumping effect. In Figure 5 the active area for the molded geometry with different materials is shown in comparison with a flat geometry. The area also extends to the decrease in operating pressure. The PTFE membrane showed a less maximum value of the Von Mises stress in comparison with PVDF membrane. This result is very important in order to assess the reliability of the membrane and the ability to trigger cracks in the central area and the connection between the stem and diaphragm

Effect of different chamber-diaphragm geometries: In Figure 6 the different pump characteristic curves for the considered geometries are shown assuming that the pumping cycles are identical. The numerical curve obtained with the standard molded diaphragm is similar to the experimental characteristic curve at the high backpressure. At the lower pressure, the numerical curve deviates from the experimental one because it was impossible to set the inlet pressure constant during the experiment. The overestimation of the experimental data is due to the spurious effect (bad reproduction of the pumping cycle, possible leakage, recirculation etc etc), which degrades performance during the real operation. The optimized molded-upgrade diaphragm shows a better performance compared to the actual molded and flat diaphragm. The connecting channels also greatly influence the motion of the fluid (see Figure 7). The increase of vorticity is followed by a generation of smaller turbulent scales and a faster energy cascade. A high vorticity is also index of non-stationarity motion. The presence of different scales and non-stationarity of the motion are therefore specific characteristics and precursors of the turbulence level of the fluid. This parameter is particularly high inside the channels, which means that the size and the shape of these channels should be subjected to further optimization (in particular of the ratio D/L with diameter D and length L). As the result of a variation of ± 20% of the channels diameter, a variation of the modulus of the vorticity of -10% and +14% has been obtained. For the purpose of a reduction of vorticity the diameter of the channels (D in Figure 4) should be increased in concomitance with optimizations previously discussed.

Result with different working fluid: A simulation with different working fluid has been performed. The results, in terms of the characteristic curve, for the molded-upgrade diaphragm are shown in Figure 8. The effect of the viscosity are clearly more marked at the higher pressure

Conclusion: A numerical modelling and performance optimization study of a diaphragm pump for drug infusion was developed. The model is able to replicate the pumping cycle (400ms) and also to provide indications about the variation of pumping performance as consequence of the variation of the geometry of the chamber-diaphragm system, materials and operating conditions. The optimal design for improvement of the pump performance is provided by using PTFE diaphragm with a molded-upgrade shape.

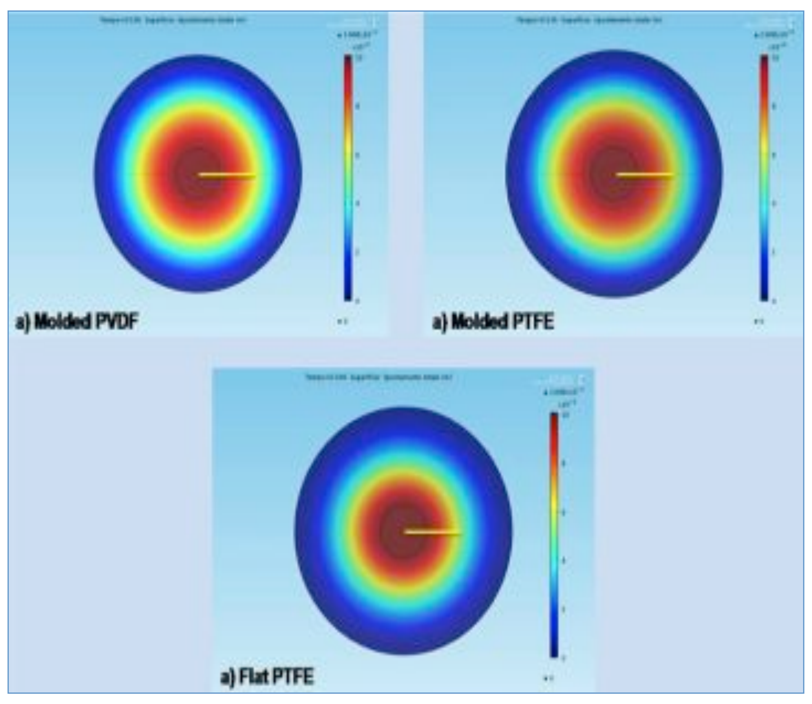

Figure 5. Active area for different diaphragm (standard molded) materials: PVDF (top left) PFTE (top right) compared to a flat PTFE diaphragm (bottom).

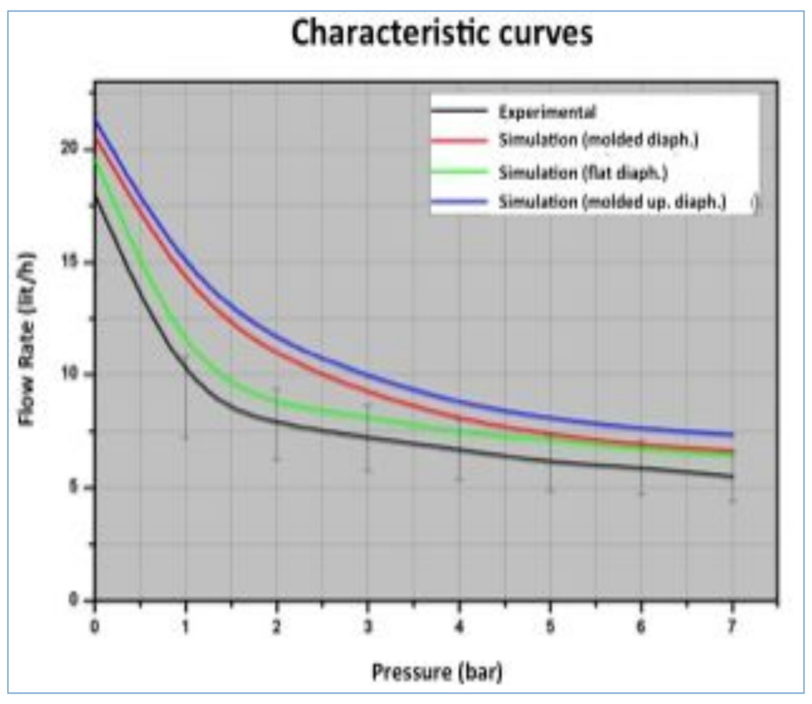

Figure 6. Characteristic curves for different standard molded, flat and molded-upgrade diaphragm compared to the experimental data.

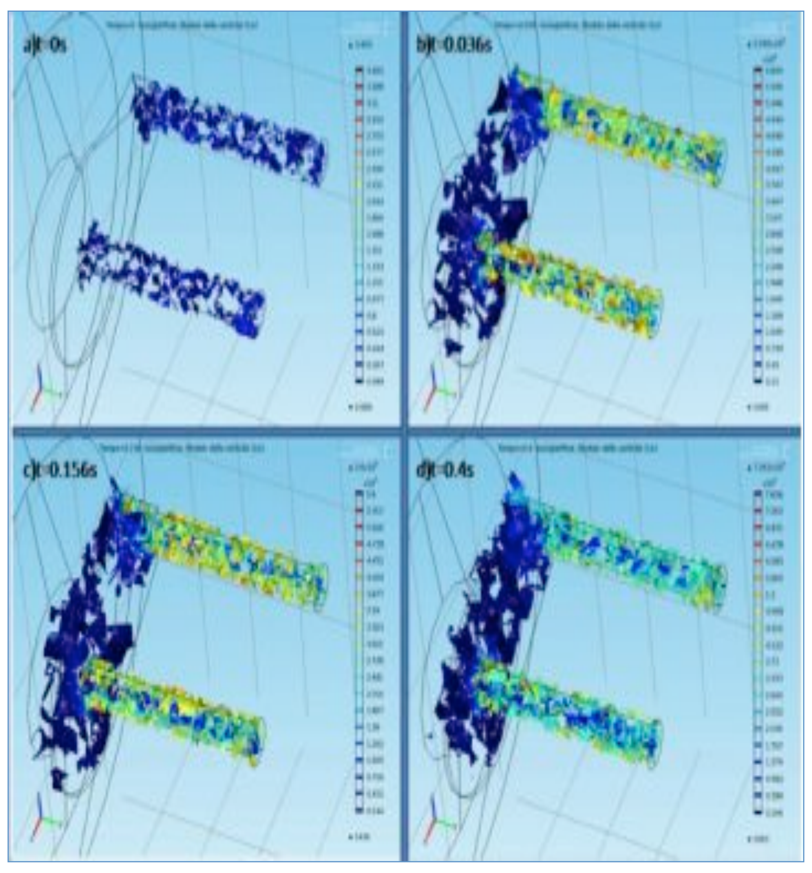

Figure 7. Vorticity field inside the pumping chamber (0s-0.036s-0.156s-0.4s).

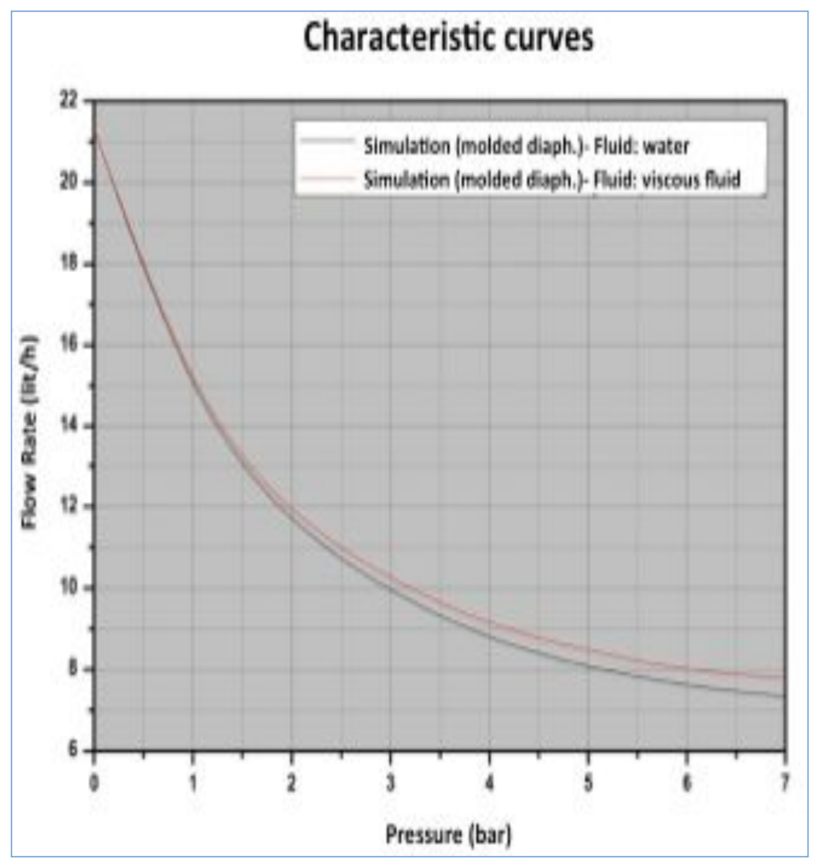

Figure 8. Characteristic curves for different standard working fluid: water and viscous fluid

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