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Three-Dimensional Finite Element Modeling of a Viscous Fluid Flowing through an External Gear Pump

Vincent G. de Bie, Luc S.D.P. Luijten, Martien A. Hulsen,* and Patrick D. Anderson

An external gear pump is a relatively simple and inexpensive pump, that is used in a variety of production systems. Numerous works have studied the external gear pump using numerical simulations; however, typically low-viscosity fluids and turbulent flow conditions are considered. Previous work of the authors focused on predicting the output fluctuation and the volumetric efficiency of an external gear pump processing high-viscosity fluids using a 2D representation. For certain conditions, backflow through all clearances could occur, resulting in a drop in volumetric efficiency. This calls for a full 3D model. Furthermore, high residence time zones are observed in the inflow channel of the pump. The 3D shape of these zones is still unknown. The aim of this work is to investigate the effect of the axial clearances on the performance of the external gear pump. A 3D mesh is generated by extruding the 2D mesh in the third direction, resulting in prism elements. This reduces the required number of elements and therewith makes the simulations computationally feasible. Introducing the axial clearances results in a lower efficiency compared to the 2D simulations. With particle tracking, the high residence time zones in the inflow channel are visualized in the 3D simulations.

1. Introduction

External gear pumps are often used in fluid transport systems, processing fluids like, for example, water, oils, chemical additives, resins, polymers, or solvents. These pumps are compact and simple, but can work at high pressures and throughputs. In the pump, the fluid is transported in the inter-teeth volumes from a lower pressure at the inflow channel to a high pressure at the outflow channel. The performance of the external gear pump is therefore strongly determined by the tightness of the clearances. These clearances determine to what value the back pressure, that is, the pressure behind the pump can rise before the volumetric efficiency of the pump drops due to significant backflow of fluid through these clearances.

Many numerical studies[1–29] focused on understanding and predicting the efficiency of an external gear pump. Most of these studies used Newtonian fluids[1–17] and turbulent flow conditions.[1–14] For the extrusion of non-Newtonian fluids, the works are limited. Rituraj and Vacca[28] studied shear-thinning fluids using a lumped parameter model. They concluded that increasing shear-thinning behavior results in a lower efficiency of the external gear pump. Strasser[29] used a CFD simulations with non-Newtonian fluids to analyze the mixing quality.

The amount of numerical works on external gear pumps that take into account the third dimension is very limited. 3D numerical simulations of an external gear pump with decompression slot and meshing contact point were developed by Castilla et al.,[30] where significant differences were observed with respect to 2D simulations. Yoon et al.[31] used the immersed solid method for their 3D numerical simulations. The simulations were performed for extremely high rotation speeds, in the order of 10,000 rpm. Their work showed that in terms of obtaining maximum flow rate, the radial and the axial clearance are the dominant geometric parameters. Corvaglia et al.[31,32] compared 3D CFD simulations to experiments, and satisfactory agreement was found for the pressure amplitudes at the pump delivery.

In our previous study,[33] a 2D numerical simulation of an external gear pump is developed. Similar effects on the output of the pump were observed for decreasing the rotation speed, decreasing the viscosity or increasing the pressure difference. When plotting the volumetric efficiency against the so-called Hersey number, that is, rotation speed times viscosity divided by pressure difference, a single pump curve appeared. For low values of the Hersey number, a drop in volumetric efficiency is observed. This is also shown for shear-thinning fluids, where the viscosity at the effective shear rate is used. The drop in efficiency is faster, that is, in a smaller range of the Hersey number for more shear-thinning fluids. Next to the pump curves, our previous study[33] showed zones with a high residence time in the inflow channel of the external gear pump.
In external gear pumps, an axial clearance is present besides the previously studied radial clearance. As shown in Figure 1, it is expected that three types of fluid flows can be present in the opposite direction as the flow direction. Depicted in blue is the backflow through the radial clearance. The green arrow is the backflow between the gears. Here, inefficient emptying of the interteeth volumes can also play a role. The last type, shown in red, is backflow through the axial clearance. For low values of the Hersey number, fluid probably also starts to flow back through this axial clearance, therewith decreasing the volumetric efficiency even further compared to the 2D simulations.

In this research, the flow of viscous fluids through an external gear pump is numerically studied using the finite element method (FEM). A 3D representation of an external gear pump is used with the rotation of both gear imposed. Local mesh refinement, based on the respective distance between boundaries, is required to accurately capture the tight radial clearances in the pump. Extrusion is used to transform the 2D mesh with triangular elements into a 3D mesh with prism elements. In this work, the 3D case is thus studied to determine for what conditions, that is, material and processing parameters, the third dimension is crucial for an accurate output prediction. The aim is to study the relative importance of the radial and axial clearance using the numerical simulations of the external gear pump. A suitable method to visualize the high residence time zones in the 3D simulations is to use particle tracking to characterize the process of mixing.\textsuperscript{[34–38]}

2. Problem Definition and Governing Equations

The flow of a viscous fluid through an external gear pump is investigated using fully resolved 3D simulations. Due to symmetry, only half of the external gear pump needs to be modeled. A schematic representation of the geometry of the pump is shown in Figure 2, whereas the dimensions are given in Table 1. Similar as was done in the previous work,\textsuperscript{[33]} a resistance channel is added behind the exit of the pump to mimic the resistance that is present due to everything behind the pump. The length of this channel can be varied to change the back pressure of the gear pump.

In practice, the rotation of one gear is imposed by a motor and, by means of contact, this gear propels the other gear. Modeling such a dynamic point is complex, and solely results in an improved description of the flow locally. Therefore, no contact point is modeled in our simulations, and the rotation is imposed for both gears. For this reason, a certain angle difference $\Delta \theta$ between both gears needs to be set. To limit the computational cost of the 3D simulations, the angle difference is chosen to be the angle of half a tooth:

$$\Delta \theta = \frac{2\pi}{N_t}$$

where $N_t$ is the number of teeth. The resulting minimum distance between the gears is approximately 200 $\mu$m, which is relatively small compared to the 50 mm tip radius of the gears.

2.1. Governing Equations

The mass and momentum balance are used to describe the flow of the fluid. It is assumed that the fluid is incompressible and that no body forces are present. Furthermore, inertia is neglected due to the high viscosity fluids that are considered. The resulting balance equations are given by:

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega$$

$$\nabla \cdot \mathbf{F} = 0 \quad \text{in } \Omega$$

$$\mathbf{F} = -\nabla p + \mu \nabla^2 \mathbf{u}$$

where $\mathbf{F}$ is the force per unit volume, $p$ the pressure, $\mu$ the dynamic viscosity, and $\nabla^2$ the Laplacian operator.
Figure 2. Schematic representation of the dimensions of the external gear pump (left and right), and its gears (middle).

Table 1. The dimensions of the 3D representation of the external gear pump.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Symbol</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height inlet</td>
<td>(H_{in})</td>
<td>50</td>
<td>mm</td>
</tr>
<tr>
<td>Length inlet</td>
<td>(L_{in})</td>
<td>25</td>
<td>mm</td>
</tr>
<tr>
<td>Clearance gear-gear</td>
<td>(\delta_{g})</td>
<td>0.5</td>
<td>mm</td>
</tr>
<tr>
<td>Radial clearance</td>
<td>(\delta_{r})</td>
<td>1.0</td>
<td>mm</td>
</tr>
<tr>
<td>Height outlet</td>
<td>(H_{out})</td>
<td>25</td>
<td>mm</td>
</tr>
<tr>
<td>Length outlet</td>
<td>(L_{out})</td>
<td>25</td>
<td>mm</td>
</tr>
<tr>
<td>Width casing</td>
<td>(W)</td>
<td>50</td>
<td>mm</td>
</tr>
<tr>
<td>Axial clearance</td>
<td>(\delta_{a})</td>
<td>1</td>
<td>mm</td>
</tr>
<tr>
<td>Number of teeth</td>
<td>(N_{t})</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Tip radius</td>
<td>(R_{t})</td>
<td>50</td>
<td>mm</td>
</tr>
<tr>
<td>Pressure angle</td>
<td>(\phi)</td>
<td>25</td>
<td>(^{\circ})</td>
</tr>
<tr>
<td>Fillet radius</td>
<td>(R_{f})</td>
<td>5.0</td>
<td>mm</td>
</tr>
</tbody>
</table>

\[-\nabla p + \nabla \cdot \mathbf{\tau} = 0 \quad \text{in } \Omega \quad (3)\]

where \(\mathbf{u}\) is the velocity vector, \(p\) the pressure, and \(\mathbf{\tau}\) the extra stress tensor. Many fluids, such as polymer melts, display non-Newtonian behavior. For this reason, a generalized Newtonian model is used:

\[\mathbf{\tau} = 2\eta(\dot{\gamma})\mathbf{D} \quad (4)\]

where \(\eta(\dot{\gamma})\) is the viscosity function, \(\dot{\gamma} = \sqrt{2\mathbf{D} \cdot \mathbf{D}}\) the shear rate, and \(\mathbf{D} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^{\top})/2\) the rate-of-deformation tensor. Shear-thinning behavior is often observed for polymer fluids at high shear rates and can be captured using a Carreau model. This model, with an infinite shear viscosity equal to zero, is given by:

\[\eta(\dot{\gamma}) = \frac{\eta_0}{\left[1 + (\dot{\gamma}/\lambda)^2\right]^n} \quad (5)\]

where \(\eta_0\) is the viscosity at zero shear rate and \(n\) the power law index. The value of \(\lambda\) controls the shear rate for the transition from Newtonian to shear-thinning behavior. Three values for the power law index \(n\) are studied: 1, 0.6, and 0.15. A value of 1 for the power law index results in Newtonian behavior, whereas decreasing the power law index results in stronger shear-thinning behavior. The viscosity of the fluids is matched at the effective shear rate, which is the shear rate between the tooth tips and the casing. This shear rate is defined as:

\[\dot{\gamma}_{\text{eff}} = \frac{\omega R_t}{\delta_r} \quad (6)\]

where \(\omega\) is the rotation speed, \(R_t\) the tip radius, and \(\delta_r\) the radial clearance. A value of 1 rad s\(^{-1}\) is used for the rotation speed in all simulations performed in this study, resulting in an effective shear rate of 50 s. The resulting parameters for the fluids are given in Table 2.

Table 2. The values of the parameters in the Carreau model for the three considered fluids.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Fluid 1</th>
<th>Fluid 2</th>
<th>Fluid 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(n)</td>
<td>-</td>
<td>1</td>
<td>0.6</td>
<td>0.15</td>
</tr>
<tr>
<td>(\eta_0)</td>
<td>Pa s</td>
<td>(1 \times 10^4)</td>
<td>(1.2 \times 10^5)</td>
<td>(1.97 \times 10^6)</td>
</tr>
<tr>
<td>(\dot{\gamma})</td>
<td>s</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>

2.2. Boundary Conditions

As can be seen in Figure 2, the boundaries of the problem are denoted by \(\Gamma\). In fluid transport systems, the filling of the external gear pump can be performed by a single-screw extruder. Therewith, the extruder generates a certain entry pressure for the gear pump. For this reason, the pressure \(p_{in}\) at the inlet of
the pump ($\Gamma_{in}$) is set. Also, it is assumed that the flow is fully developed. The resulting boundary conditions are:

$$t_x = p_{in}, \quad u_y = 0, \quad u_z = 0 \quad \text{on} \quad \Gamma_{in}$$  \hspace{1cm} (7)

where $t = \sigma \cdot n$ is the traction vector with $\sigma = -p I + \tau$ the Cauchy stress tensor and $n$ the outwardly directed normal vector. The entry pressure $p_{in}$ is set to 0 bar for all simulations in this work. No slip is assumed at the casing ($\Gamma_{casing}$). Thus, the boundary condition for the casing is given by:

$$u = 0 \quad \text{on} \quad \Gamma_{casing}$$  \hspace{1cm} (8)

The casing includes the casing of the gear pump and the walls of the resistance channel. As modeling contact is complex and beyond the scope of this study, both gears are rotated with a certain rotation speed. The velocity of the fluid at the gear boundaries ($\Gamma_{gears}$) is equal to the velocity of the gears itself, since we assume no slip. The boundary condition for the gears thus becomes:

$$u = o r e_\theta \quad \text{on} \quad \Gamma_{gears}$$  \hspace{1cm} (9)

where $r$ is the distance to the gear center and $e_\theta$ the unit vector tangential to a cylinder with the origin in the gear center and radius $r$. Due to symmetry, there is no velocity in the $z$-direction at the symmetry plane ($\Gamma_{sym}$), and the traction is zero in the other directions:

$$t_x = 0, \quad t_y = 0, \quad u_z = 0 \quad \text{on} \quad \Gamma_{sym}$$  \hspace{1cm} (10)

A fully developed flow and no horizontal traction are assumed at the outlet of the resistance channel ($\Gamma_{out}$). This results in the following boundary conditions:

$$t_x = 0, \quad u_y = 0, \quad u_z = 0 \quad \text{on} \quad \Gamma_{out}$$  \hspace{1cm} (11)

3. Numerical Method

In the numerical simulations, the finite element method (FEM) is used to solve the governing equations. Therefore, discretization of space is needed. Only half of the external gear pump is meshed due to symmetry. Static and moving boundaries are present in the problem, and thus a new mesh needs to be generated for every time step. The authors are aware of methods like fictitious domain method, immersed boundary method or XFEM, but due to the very narrow gap regions prefer a body-fitted method. A mesh is generated containing prism elements. Quadratic/biquadratic interpolation ($P_2Q_2$) for the velocity is employed, whereas the interpolation of pressure is linear/bilinear ($P_1Q_1$). The simulations are performed using a direct solver, the Pardiso solver integrated in the MKL library, on four parallel cores.

The meshing procedure is shown in Figure 3. For the first part of the mesh, a 2D mesh of the external gear pump with local mesh refinement is generated, (a). This mesh consists of triangular isoparametric elements. The meshing procedure for this 2D mesh is based on the work of Mitrias et al.$^{[39]}$ and is discussed in earlier work of the authors.$^{[33]}$ In principle, the local element size is determined by the respective distance between boundaries. This mesh is extruded in the third direction, (b), resulting in a mesh with prism elements. A gradient in the extrusion thickness of the layers of prism element is used, resulting in a large thickness at the symmetry plane and a smaller thickness at the other side. In Table 3, the thickness ratio between the
of 2δ/Δ = 0.02, eight layers over the gear width, and a radial clearance of δ/R = 0.02 at θ = 0°.

<table>
<thead>
<tr>
<th>Number of nodes</th>
<th>591 590</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of elements</td>
<td>131 772</td>
</tr>
<tr>
<td>Number of degrees of freedom</td>
<td>1 856 910</td>
</tr>
<tr>
<td>Ratio thickest/thinnest layer</td>
<td>192</td>
</tr>
</tbody>
</table>

thickest and the thinnest layer is given for one specific situation.

For the second part of the mesh, the axial clearance, the space in the gears in the 2D mesh needs to be filled with elements. In order to do this, the boundaries of the gears are extracted from the 2D mesh. With these boundaries, 2D meshes of the gears are generated with a larger element size in the center, (c). The 2D meshes of the gears are merged with the 2D mesh of the pump, (d). The resulting mesh is then extruded in the third direction to get a 3D mesh of the axial clearance of the external gear pump, (e). A uniform extrusion thickness is used for every layer of prism elements in this part of the mesh. The smallest layer in the 3D mesh of (b), has the same thickness as the layers in the mesh of (e). When choosing one layer in the clearance, the amount of layers in the mesh of (b) needs to be at least two for this to be possible. Thus, the amount of layers spanning the gear width is chosen to be twice the amount of layers spanning the axial clearance. Merging the two 3D meshes, (b,e), results in the 3D mesh of the pump, (f). A resistance channel is added behind the exit of the gear pump, (g), to mimic the resistance of everything that is normally present behind the pump. An indication of the size of the resulting mesh is given in Table 3 for one specific mesh.

4. Results

The results of this work are twofold: the effect of the clearances on the output is studied and the high residence time zones are visualized using particle tracking.

4.1. Throughput Pump

In this section, the mesh convergence is studied to determine the amount of layers of prism elements needed to get an accurate solution. Thereafter, the flow rate, the pressure difference, and the efficiency of the 3D simulations are compared to the 2D case.

4.1.1. Mesh Convergence

The accuracy of the simulation is assured using a convergence study. The problem is time dependent in terms of the rotation of the gears, that is, due to the geometry. At a fixed time, the accuracy of the solution is independent of the time discretization, and thus the time step can be freely chosen. A time step that results in 1° rotation of the gears is used in the simulations of this section. For the particle tracking, a separate time convergence study is performed in Section 4.2.1.

The spatial convergence of the 2D mesh has already been studied in our previous work.[33] In this work, we focus on the amount of layers needed to get an accurate output prediction. The velocities and pressures on the plane denoted by the gray dashed line in Figure 2 are sampled on a grid of 1000x1000 points. The maximum norm is used to determine the errors of the output:

\[
\epsilon_u,i = \frac{\text{max}|u_i - u_{\text{ref}}|}{\text{max}(u_{\text{ref}})}
\]

\[
\epsilon_p,i = \frac{\text{max}|p_i - p_{\text{ref}}|}{\text{max}(p_{\text{ref}})}
\]

where subscript i refers to the number of layers spanning the axial clearance, and subscript “ref” refers to the refined mesh with 25 layers spanning the axial clearance. Note, that the number of layers spanning the gear width is chosen to be twice the amount of layers spanning the axial clearance, as was discussed in Section 3. The mesh convergence study is performed for the Newtonian fluid, that is, \( n = 1 \). The resulting errors of the output are plotted in Figure 4. These plots show that the error decreases when increasing the number of layers. The error of the pressure almost never exceeds our convergence criterion of 1%. For the velocity, at least four layers need to span the axial clearance for an error below the criterion. Therefore, a 3D mesh is used with eight layers spanning the gear width and four layers spanning the axial clearance. Note, that the number of nodes across the width is twice the number of layers plus one.

4.1.2. Flow Rate and Pressure Difference

The output of the gear pump is obtained in terms of flow rate \( \dot{Q} \) and mean pressure difference \( \Delta p \). The flow rate is computed by numerical integration of the horizontal velocity over the exit of the pump, denoted by the black dashed line in Figure 2. The flow rate is compared to the theoretically achievable flow rate. The 2D theoretical flow rate is obtained by subtracting the area of the side wall of a gear from a circle with the tip radius and multiplying by the number of rotations per second (\( \omega_2/2\pi \)) and the number of gears. For the 3D case, this is multiplied by the width \( W \). In the computation of the theoretical flow rate, the clearances are assumed to be zero. The mean pressure difference is computed by:

\[
\Delta p = \frac{1}{n_p} \sum_{i=1}^{n_p} p_i - p_m
\]

where \( n_p \) is the number of sample points over the outlet line (2D) or plane (3D).

First, the influence of changing the radial clearance is studied for a Newtonian fluid using our 2D simulations.[31] The results are shown in Figure 5. The presented flow rate is obtained from the 2D simulations by multiplying by the width \( W \). As is observed before, the output fluctuates with a frequency that is related to the number of teeth of a gear. The observed fluctuations is way smoother as the frequency spectrum sometimes observed in experiments,[2,3,8,12,18,21,29] which can be the result of many factors. In experiments, the material behavior is often dependent on shear rate, temperature, pressure, and/or even time.
Figure 4. The relative error of the output for the surface at a quarter of the outflow channel with respect to the reference mesh (25 layers), for the external gear pump with $2\frac{\delta_a}{W} = 0.02$, $\frac{\delta_r}{R} = 0.02$, $\omega = 1$ rad s$^{-1}$, and $L_{\text{res}} = 30$ mm, processing a Newtonian fluid ($n = 1$) with $\eta_0 = 10^4$ Pa s, as a function of the number of layers of prism elements in the axial clearance: a) horizontal velocity $u_x$, and b) pressure $p$.

Furthermore, the inflow pressure of the pump is assumed constant, which is quite challenging in experiments. The axes of the gears are also placed in hydrodynamic bearing, resulting in radial clearances that fluctuate in size. Finally, even wall slip could be present in the external gear pump.

For the same length of the resistance channel, a larger radial clearance results in a higher flow rate and an increase of the pressure difference over the pump. A larger clearance increases the amount of fluid being dragged along in the radial clearance due to the rotation of the gears, resulting in a higher flow rate. The pressure difference is mainly determined by the resistance of the channel behind the exit of the pump:

$$\Delta p = QR$$

where $R$ is the resistance. For the same dimensions of the resistance channel, and thus the same resistance, a higher flow rate results in an increase of the pressure difference.

In Figure 5, the output for a 2D case is compared to the 3D case with a small axial clearance, $2\frac{\delta_a}{W} = 0.004$. The values of the pressure difference are larger in 3D as for the 2D case, despite the equal resistance channel length. This can be explained using the resistance of this channel. The 2D case is similar to an infinite parallel-plate channel, where for a Newtonian fluid the resistance is given by:

$$R = \frac{12\mu L_{\text{res}}}{H_{\text{out}}^3 W}$$

assuming a width of $W$. The 3D case is a channel with a rectangular cross-section, and then the resistance can be approximated by:

$$R = \frac{12\mu L_{\text{res}}}{H_{\text{out}}^3 W \left[ 1 - 0.630 \frac{H_{\text{out}}}{W} \right]}$$

Clearly, the resistance of the 3D channel is larger as for the 2D case. Therefore, the same flow rate would result in a higher pressure for the 3D case. At these conditions, the larger pressure difference in the 3D simulations does not seem to result in a significant drop of the flow rate, since in 3D it is only slightly lower. This slightly lower flow rate could also be explained by the fact that the width of the gears is defined as $(W - 2\delta)$, which makes the width smaller when an axial clearance is present. This also results in a lower flow rate for the 3D case.
Figure 6. The output of the 2D pump with $\delta_r / R = 0.02$ and the output of the 3D pump with $\delta_r / R = 0.02$ and $2\delta_a / W = 0.004$, for $\omega = 1 \text{ rad s}^{-1}$ and $L_{\text{res}} = 300 \text{ mm}$, processing a Newtonian fluid ($n = 1$) with $\eta_0 = 10^4 \text{ Pa s}$, as a function of rotation angle of the gears: a) flow rate and b) mean pressure difference.

Figure 7. The output of the 3D external gear pump with $\omega = 1 \text{ rad s}^{-1}$, $L_{\text{res}} = 300 \text{ mm}$, and $\delta_r / R = 0.02$ for different sizes of the axial clearance, processing a Newtonian fluid ($n = 1$) with $\eta_0 = 10^4 \text{ Pa s}$, as a function of rotation angle of the gears: a) flow rate and b) mean pressure difference.

With the help of the 3D simulations, the influence of changing the axial clearance on the output is studied, as shown in Figure 7. A higher flow rate and an increase of the pressure difference over the pump are observed for simulations using the same resistance channel length, but an increasing axial clearance. Dragging along fluid is less important for the axial clearance, since fluid is dragged along from the entry to the exit but also vice versa. A larger clearance then mostly results in a higher chance of backflow occurring, which decreases the flow rate. Furthermore, increasing the axial clearance results in a lower flow rate due to the decreasing width of the gears, since the width of the gears is defined as $(W - 2\delta_a)$. A lower flow rate results in a decrease of the pressure difference. For a large axial clearance, not only the values of the output seem to decrease, but also the amplitude of the output fluctuations decreases quite significantly.

In our previous work,\textsuperscript{[33]} it was observed that for the same pressure difference over the external gear pump, a stronger shear-thinning fluid results in a smaller fluctuation in the pressure difference over the pump. Figure 8 shows what the effect is of introducing an axial clearance on the influence of the amount of shear-thinning behavior on the output of the pump. The same decrease of the amplitude of the pressure-difference fluctuation with increasing amount of shear-thinning behavior is observed. Furthermore, the flow-rate fluctuation gets a sharper shape at its minimum value for the strongly shear-thinning fluid. The slight decrease of the flow rate when lowering the value of $n$ can be partly attributed to the fact that the mean value of the pressure difference slightly increases. Besides that, there is a higher chance that the shear-thinning fluids flow back through the clearances.

4.1.3. Efficiency

The volumetric efficiency is defined by the ratio of the flow rate of the external gear pump $Q$ and the theoretically achievable flow rate of the pump $Q_{\text{theo}}$, that is,

$$\eta_{\text{vol}} = \frac{Q}{Q_{\text{theo}}} \times 100$$  \hspace{1cm} (18)

if expressed as percentage. The theoretical flow rate can be computed using the dimensions of the gears:

$$Q_{\text{theo}} = (\pi R^2 - A_{\text{gear}})(W - \delta_a) \frac{\alpha}{\pi}$$  \hspace{1cm} (19)
The output of the 3D external gear pump with $\omega = 1 \text{ rad s}^{-1}$, $\Delta p \approx 100 \text{ bar}$, $\delta_r/R = 0.02$, and $2\delta_a/W = 0.004$, processing fluids with different power law indices, but a matched viscosity of $\eta_0 = 10^4 \text{ Pa s}$ at the effective shear rate, as a function of rotation angle of the gears: a) flow rate and b) mean pressure difference.

The volumetric efficiency of the 2D external gear pump with $\omega = 1 \text{ rad s}^{-1}$ and different radial clearances, processing a Newtonian fluid ($n = 1$) with a constant viscosity $\eta_0 = 10^4 \text{ Pa s}$ as a function of the Hersey number: a) $\eta_{\text{vol},1}$ and b) $\eta_{\text{vol},2}$.

or the dimensions of the casing:

$$Q_{\text{theo},2} = \left(\pi (R + \delta_r)^2 - A_{\text{gear}}\right) W W$$

where $A_{\text{gear}}$ is the area of the side wall of a gear. For the first definition of $Q_{\text{theo},2}$, the 3D flow rate is obtained from 2D simulations using a multiplication with $(W - \delta_r)$. For $Q_{\text{theo},2}$, it is multiplied by the width of the casing $W$. The Hersey number is defined as:

$$\text{He} = \frac{\mu \omega}{\Delta p}$$

where $\mu$ is the Newtonian viscosity. By changing the length of the resistance channel, the pressure difference over the pump is varied, resulting in different values of the Hersey number.

The pump curves, that is, the volumetric efficiency versus the Hersey number, are shown for both definitions of the theoretical flow rate in Figure 9 for the 2D case. For both definitions, a larger clearance leads to a faster drop in efficiency at low values of the Hersey number. At higher values of the Hersey number, the efficiency of Figure 9a shows that when the radial clearance is higher, more material from the clearance is dragged along with the gears, resulting in a higher efficiency. For $\eta_{\text{vol},1}$, the tip radius of the gear is used to determine the theoretical flow rate, which means that it is independent of the radial clearance. In the case of $\eta_{\text{vol},2}$, the radius of the casing is used for the theoretical flow rate, resulting in a higher value for a larger axial clearance. For this reason, the efficiency of Figure 9b does not display a higher efficiency at a higher Hersey number for a large clearance, but the highest efficiency is obtained for the smallest radial clearance.

Figure 10 shows the pump curves for the 3D case. The dashed gray line is the 2D pump curve for $\delta_r/R = 0.02$, as this radial clearance is used for the 3D simulations. For a small axial clearance, the difference between the 2D and the 3D simulations are negligible. An increase in axial clearance results in a lower efficiency and the drop in efficiency initiates at higher Hersey numbers. The effect of the radial clearance on the efficiency is significantly larger than the effect of axial clearance. On half of the gears, the horizontal velocity is positive and on the other half, it is negative. Probably, some fluid is flowing back through the axial clearance, but also some fluid is dragged along to the outflow side.

For shear-thinning fluids, the Hersey number is defined using the viscosity at the effective shear rate instead of the Newtonian viscosity. The volumetric efficiency versus the Hersey number for the three fluids with different amounts of shear-thinning behav-
Figure 10. The volumetric efficiency of 3D external gear pumps with $\delta_r/R = 0.02$, $\omega = 1\text{ rad s}^{-1}$, and different axial clearances processing a Newtonian fluid ($n = 1$) with a constant viscosity $\eta_0 = 10^4\text{ Pa s}$ as a function of the Hersey number: a) $\eta_{vol,1}$ and b) $\eta_{vol,2}$.

Figure 11. The volumetric efficiency of 3D external gear pumps with $\delta_r/R = 0.02$, $2\delta_a/W = 0.004$, and $\omega = 1\text{ rad s}^{-1}$, processing fluids with different power law indices, but a matched viscosity of $10^4\text{ Pa s}$ at the effective shear rate, as a function of the Hersey number: a) $\eta_{vol,1}$ and b) $\eta_{vol,2}$.

ior is shown in Figure 11. This study is performed for the smallest axial clearance, since this ratio between the axial and the radial clearance is most realistic for commercial external gear pumps. An increase in the amount of shear-thinning behavior results in a faster drop in efficiency at low Hersey numbers. However, no significant difference between the 2D (dashed lines) and the 3D (markers) case is observed. This would imply that for realistic clearances, the axial clearance does not play a significant role in the determination of the efficiency. Therefore, 2D simulations could be sufficient.

The velocity and viscosity in the axial clearance are visualized in Figure 12 for the fluid with the strongest shear-thinning behavior. In the middle of the domain, the horizontal velocity is most negative, pointing out that over here fluid is flowing back from the exit to the entry. So, fluid does seem to flow back through the axial clearance. However, it does not significantly influence the efficiency of the external gear pump. Next to this, small zones close to the tips of the gears are observed that show backflow of fluid. This happens close to the tip due to the lower viscosity resulting from the shear-thinning behavior.

4.2. Particle Tracking

With particle tracking, the motion of individual particles within a fluid is observed to study their trajectories. Gorodetskyi et al. studied some prototypical flows using particle tracking and Sarhangi Fard et al. a real processing flow. In this section, the high residence time zones, observed by the authors for the 2D case, are studied for the 3D case with the help of particle tracking. For this, it is assumed that the particles passively follow the flow:

$$\frac{dx_p}{dt} = u(x_p, t)$$

where $x_p$ is the position of the particle. To solve the equation above, an adaptive time step Runge–Kutta method is used. This method scales the time step using an error estimation. It is implemented that the time step is rejected when a particle leaves the domain $\Omega$, and thus a smaller time step is used such that the particle stays in the domain. The finite element simulations are solely performed using a certain fixed time step. When the Runge–Kutta solver chooses a smaller time step, the velocity fields are linearly interpolated between time steps.

4.2.1. Time Convergence

The accuracy of the particle tracking is highly dependent on the chosen time step for the finite element simulations. The time convergence of the particle position is checked by means of tracking one particle for the rotation of one tooth. This particle is po-
Figure 12. The a) horizontal velocity, b) vertical velocity, and c) viscosity in the external gear pump with $\delta_r / R = 0.02$, $2\delta_a / W = 0.004$, $\omega = 1$ rad s$^{-1}$, and $L_{res} = 2$ m, for a shear-thinning fluid ($n = 0.15$, $\eta_0 = 1.97 \cdot 10^6$ Pa s, $\lambda = 10$ s) at $\theta = 0^\circ$.

4.2.2. Two Dimensions

The 2D simulations\cite{33} are used to compare the residence time distribution with the particle positions. The high residence time zones in our previous work\cite{33} decreased in size and eventually vanished when decreasing the height of the inlet channel of the pump. In Figure 14, the result of tracking a high number of particles is shown for varying inlet height. Good agreement is found between the zones with a high residence time and the particle positions after five rotations. Particles get stuck in these high residence time zones and are not released within the simulation time. Occasionally, one of the particles at the boundary of the high residence time zones is dragged along in one of the inter-tooth volumes. For decreasing inlet height, less particles remain in the inlet channel after five rotations.

The periodicity of the velocity in the external gear pump is the rotation of one gear tooth. A Poincaré map can be obtained by superimposing the particle positions after each period.\cite{44–48} In order to do this, a closed domain needs to be mimicked. Therefore, when a particle leaves the exit of the pump, the length of the pump is subtracted from its $x$-coordinate and its $y$-coordinate is scaled with the ratio of the inlet height over the outlet height. In this way, the particle re-enters the domain at the entry. In the pump, 110 particles are randomly positioned and tracked over time. The resulting Poincaré maps after 200 periods, that is, 20 rotations, are shown in Figure 15. The same trends are observed for decreasing the height of the inflow channel of the pump. In other words, the size of the white areas in the inflow channel where no particles have been within these 20 rotations, decreases or even vanishes for a smaller height of the inflow channel.

Instead of tracking the particles which are not in the high residence time zones, we now position some particles in these zones. In Figure 16b, every color belongs to a single particle. This clearly shows that particles circle in these high residence time zones. If the particle is within the Kolmogorov–Arnold–Moser (KAM) boundary\cite{43} (red), it will circle around for an infinite time. The shapes of these particle trajectories fluctuate over time, as shown in Figure 17, but after one period, the same shape is retrieved.

$$e = \frac{\sqrt{(x - x_{ref})^2 + (y - y_{ref})^2}}{H_{in}/2}$$

where subscript “ref” indicates the reference time step. The resulting relative errors are plotted in Figure 13. A relative error of 1% is chosen as the convergence criterion. The time step belonging to $N = 144$, that is, a rotation of 0.25° per time step, gives a sufficiently accurate result. This time step is consistently used for all simulations below.
The results above showed that particle tracking is a viable option to visualize the high residence time zones in the external gear pump. It can even give some information about infinite residence times in the pump. Therefore, 3D simulations are analyzed using this method. The result of tracking 32 500 particles in a 3D simulation of an external gear pump is shown in Figure 18. It seems like, for the largest part of the domain, the 2D shapes of the high residence time zones are extruded in the third direction. Close to the side wall of the pump, the shape seems to be slightly different. One possible explanation could be that the velocity close to the side wall is small due to the no-slip boundary condition, and thus the particles did not have time to exit the inflow channel within the simulations time of five rotations.

In the histograms of Figure 19, we can clearly see the deviations in the number fraction of particles \( N_p \) in the third direction towards the side wall. The normalized coordinate \( z^* \) is used, which is zero at the symmetry plane (\( z = 0 \) mm) and one at the side wall of the casing (\( z = W/2 \)). When decreasing the size of the axial clearance, the distribution of particles over the third direction becomes slightly more uniform, but the difference is negligible. As mentioned before, the increase in the number of particles close to the wall could possibly be attributed to the limited simulations time, but could also be an effect caused by the axial clearance. For the major part of the inflow channel, the shape of the high residence time zones is an extrusion of the 2D shape. Therefore, studying these zones with 2D simulations already gives extremely valuable information.

### 5. Conclusions

This work presents 3D finite element simulations of an external gear pump processing high-viscosity fluids. In order to do this, a 2D mesh is generated with local mesh refinements that are based on the respective distance between boundaries. With the help of extrusion of the triangular elements, a 3D mesh with prism elements is generated. The velocity and pressure distribution are ob-

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**Figure 14.** The particle positions in the external gear pump with \( \omega = 1 \) rad s\(^{-1} \) and \( L_{res} = 2 \) m, for a Newtonian fluid \((n = 1, \eta_0 = 10^4 \) Pa s\) after five rotations: a) \( H_{in} = 50 \) mm, b) \( H_{in} = 35 \) mm, and c) \( H_{in} = 20 \) mm.

**Figure 15.** The Poincaré maps of the external gear pump with \( \omega = 1 \) rad s\(^{-1} \) and \( L_{res} = 2 \) m, for a Newtonian fluid \((n = 1, \eta_0 = 10^4 \) Pa s\) after 200 periods: a) \( H_{in} = 50 \) mm, b) \( H_{in} = 35 \) mm, and c) \( H_{in} = 20 \) mm.
Figure 16. The Poincaré maps of the external gear pump with $H_{in} = 50$ mm, $\omega = 1$ rad s$^{-1}$, and $L_{res} = 2$ m, for a Newtonian fluid ($n = 1$, $\eta_0 = 10^4$ Pa s) after 200 periods: a) zoom of Poincaré and b) zoom of inverted Poincaré.

Figure 17. The dynamics of a blob within the KAM boundaries of the external gear pump with $H_{in} = 50$ mm, $\omega = 1$ rad s$^{-1}$, and $L_{res} = 2$ m, for a Newtonian fluid ($n = 1$, $\eta_0 = 10^4$ Pa s) for one period: a) upper zone and b) lower zone.

Figure 18. The particle positions in the external gear pump with $2\delta_y/W = 0.004$, $\omega = 1$ rad s$^{-1}$, and $L_{res} = 3$ mm, for a Newtonian fluid ($n = 1$, $\eta_0 = 10^4$ Pa s) after five rotations: a) horizontal view and b) top right view.
Figure 19. Histograms of the distribution of the number fraction of particles in the z-direction in the external gear pump with \( \omega = 1 \text{ rad s}^{-1} \) and \( L_{\text{res}} = 3 \text{ mm} \), for a Newtonian fluid \((n = 1, \eta_0 = 10^6 \text{ Pa s})\) after five rotations: (a–c) upper zones, (d–f) lower zones; (a,d) 2\( \delta_a/W \) = 0.04, (b,e) 2\( \delta_a/W \) = 0.02, and (c,f) 2\( \delta_a/W \) = 0.004.

The histograms show the distribution of particles in the z-direction. The relative importance of the radial and the axial clearances are studied. This is done for fluids with different amounts of shear-thinning behavior.

Using 2D simulations, it is observed that for increasing radial clearance, the flow rate and the pressure difference over the pump drop. The frequency of the output fluctuation is, as observed before, related to the number of teeth of a gear. For the 3D case, a larger axial clearance also results in a lower flow rate and pressure difference over the pump. However, a significant decrease in fluctuation amplitude is observed. When increasing the amount of shear thinning, the flow rate drops slightly, whereas the amplitude of the fluctuation in pressure difference over the pump decreases significantly.

The Hersey number is changed by varying the length of the resistance channel and therewith the pressure difference over the pump. At high values of the Hersey number, the gears drag along some material, making the efficiency somewhat higher for larger radial clearances. At low values of the Hersey number, the drop in efficiency is faster for larger radial clearances. The effect of the axial clearance on the efficiency of the pump seems less pronounced as the radial clearance. Nevertheless, a larger axial clearance results in a lower efficiency for all values of the Hersey number. When using realistic values for the clearances, the extra loss in efficiency due to the axial clearance is small, even for a strongly shear-thinning fluid.

Using particle tracking, the earlier observed high residence time zones in the inflow channel of the external gear pump are visualized for a 3D situation. For our geometry of the external gear pump, it appears that the 3D shape of these zones, is to a great extent an extrusion of the 2D shape. Towards the walls of the inflow channel, an increase in the number of particles is observed. It is uncertain if this can be attributed to the introduction of an axial clearance or if this is observed due to the limited simulation time of five rotations. All in all, it could be concluded that for this geometry of the external gear pump, the extra information obtained by going to 3D does not outweigh the increase in computational cost, and thus 2D is sufficient. Note, many effects, like the effect of temperature and pressure on the fluid properties or viscoelasticity, are not taken into account in this study. These effects could also influence the efficiency of the pump or the shape of the high residence time zones.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.
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