Numerical analysis of the flow of power law fluids in coat hanger dies

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Numerical analysis of the flow of Power Law fluids in coat hanger dies
G.A.A.V. Haagh
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Eindhoven University of Technology
Department of Mechanical Engineering
Division of Engineering Fundamentals
Centre for Polymers and Composites
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This work was supervised by dr.ir. G.W.M. Peters
Summary

In polymer processing, the material flow often passes from an extruder to the next processing stage through a die. In many processes, the object is to obtain a flow of uniform shear deformation history, uniform averaged residence time, and uniform averaged exit velocity coming out of the die. The geometry of dies that meet these demands can be derived analytically for Power Law fluids in an isothermal flow; they turn out to be shaped like coat hangers.

The theoretical analysis of coat hanger dies is two-dimensional, implying that the influences of side walls and of a sudden decrease in channel height is neglected. These assumptions are tested by performing both two-dimensional and three-dimensional computations on a test problem. They prove to be correct.

The isothermal flow of material in two types of coat hanger dies is simulated numerically with the VIP program. The results of these simulations match quite well with the theoretical analysis, although some improvements might be made. Using the VIP program gives the opportunity to analyse more complex fluids, non-isothermal flows, and multicomponent flows, and to perform particle tracking on these flows. It is also possible to simulate the filling of a mould with a coat hanger die attached to it.

Although coat hanger dies have originally been developed for sheet extrusion, the aspect of uniform residence time can make them also useful for applications in reaction injection moulding processes. There they can provide uniformity of degree of conversion of the material flow entering the mould.
Nomenclature

Symbols

- $a$ manifold aspect ratio $\frac{W}{h}$ [-]
- $b$ half manifold width [m]
- $B$ dimensionless parameter $\frac{W}{b}$ [-]
- $D$ dimensionless parameter $\frac{\alpha h f_x}{b}$ [-]
- $f_p$ pressure correction factor [-]
- $h$ slit height [m]
- $H$ initial manifold height [m]
- $n$ power law exponent [-]
- $p$ pressure [Pa]
- $Q$ flow rate $[m^3/s]$ 
- $\Delta t$ residence time [-]
- $u, v, w$ velocity in $x, y, z$ direction [m/s]
- $\bar{v}$ average velocity [m/s]
- $W$ manifold width [m]
- $\eta$ viscosity [Pa.s]
- $\dot{\gamma}$ shear rate $[s^{-1}]$

Subscripts
- $m$ with respect to manifold
- $s$ with respect to slit region
- $w$ with respect to wall

Superscripts
- $o$ reference value
# Contents

1 Introduction 4

2 Theoretical analysis of a coat hanger die 5
   2.1 Requirements for a coat hanger die 5
   2.2 Determining the die geometry 5

3 Verification of some assumptions on the coat hanger die 11
   3.1 Method of verification 12
   3.2 A criterion for comparison 14
   3.3 Results on test problems 15
      3.3.1 Test on side wall effects 15
      3.3.2 Test on effects of height transition 15
   3.4 Conclusions 15

4 Coat hanger die simulations 23
   4.1 Coat hanger of constant manifold width 23
   4.2 Coat hanger of constant manifold aspect ratio 24

5 Conclusion 34

# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Coat hanger die distribution system. (After Winter and Fritz, 1986.)</td>
</tr>
<tr>
<td>2</td>
<td>Shape factor ( f_p ) as a function of aspect ratio ( \frac{W}{H} ). (After Tadmor and Gogos, 1979.)</td>
</tr>
<tr>
<td>3</td>
<td>Geometries for coat hanger dies of constant manifold width (left) and constant manifold aspect ratio (right): manifold contours (above) and heights (below). ( (D = \frac{W}{b}, B = \frac{W f_p h}{s H}) ).</td>
</tr>
<tr>
<td>4</td>
<td>Mesh for SEPRAN calculations on test geometry.</td>
</tr>
<tr>
<td>5</td>
<td>Mesh for VIP calculation on test geometry.</td>
</tr>
<tr>
<td>6</td>
<td>Intersection at ( z = 0.5 \text{ mm} ) (above) and at ( x = 25 \text{ mm} ) (below) of SEPRAN velocity field in test geometry with side wall effects.</td>
</tr>
<tr>
<td>7</td>
<td>Intersection at ( z = 0.5 \text{ mm} ) of SEPRAN velocity field in test geometry without side wall effects.</td>
</tr>
<tr>
<td>8</td>
<td>SEPRAN particle tracks from exit to entry in test geometry without side wall effects (time span between two small circles on a track is 2 seconds).</td>
</tr>
<tr>
<td>9</td>
<td>Summary of particle tracking results on SEPRAN test problems with and without side wall effects, and on VIP test problem.</td>
</tr>
<tr>
<td>10</td>
<td>VIP time labels for test geometry.</td>
</tr>
<tr>
<td>11</td>
<td>VIP y-labels (in midplane) for test geometry.</td>
</tr>
<tr>
<td>12</td>
<td>Mesh for coat hanger die of constant manifold width.</td>
</tr>
<tr>
<td>13</td>
<td>Coat hanger die of constant manifold width ( (n = 0.4) ): height (above) and pressure distribution (below).</td>
</tr>
<tr>
<td>14</td>
<td>Coat hanger die of constant manifold width ( (n = 0.4) ): injection time (above) and ( z )-labels (below) in midplane.</td>
</tr>
</tbody>
</table>
Coat hanger die of constant manifold width \((n = 0.4)\): wall shear rate distribution.

Coat hanger die of constant manifold width \((n = 0.7)\): midplane injection time labels (above) and wall shear rate distribution (below).

Mesh for coat hanger die of constant manifold aspect ratio.

Coat hanger die of constant manifold aspect ratio \((n = 0.4)\): height (above) and pressure distribution (below).

Coat hanger die of constant manifold aspect ratio \((n = 0.4)\): injection time (above) and \(x\)-label (below) in midplane.

Coat hanger die of constant manifold aspect ratio \((n = 0.4)\): wall shear rate distribution.

List of Tables

1. Geometrical data for coat hanger test geometry. ........................................ 12
2. Parameters for simple 3-D Stokes flow calculation. ................................. 15
3. SEPRAN particle tracking results on test geometry with side wall effects ... 21
4. SEPRAN particle tracking results on test geometry without side wall effects. 21
5. VIp particle tracking results on test geometry without side wall effects ....... 22
7. Material and computational parameters for coat hanger die simulation. .... 23
8. Geometrical data for coat hanger die of constant manifold aspect ratio. (Based on Winter and Fritz, 1986.) ......................................................... 25
1 Introduction

In polymer processing, the polymer material is often transported from an extruder to the actual processing stage through a die, which has to take care of the distribution of the material flow that is needed for further processing. These dies can induce non-uniformity in the deformation history of the material leaving the die exit, thereby causing the polymer to be inhomogeneous with respect to its mechanical and thermal properties. Uniformity is defined here with respect to the position along the die width; uniformity in the direction of die height is obviously not possible. Furthermore, if the material is reactive, as in reaction injection moulding, it may enter the mould having different degrees of conversion due to differences in die residence time, causing a non-uniform material flow in the mould. To avoid such problems, the die should be designed as to enable a proper distribution of the material flow without introducing inhomogeneity.

After the geometry of a die that meets these demands has been derived through theoretical analysis, it is checked whether the VIP finite element package will produce numerical results that coincide with analytical results.
2 Theoretical analysis of a coat hanger die

2.1 Requirements for a coat hanger die

For the extrusion of sheets, a die is needed to convert the channel flow of material coming out of the extruder into a planar flow. In order to minimise the variance in properties and thickness along the sheet width, a uniform deformation history is desirable. Therefore, Winter and Fritz (1986) state that a properly designed die for the extrusion of sheets has to meet the following demands:

1. The polymer melt is to be distributed completely and uniformly over the die exit (i.e. a uniform exit velocity and a uniform average residence time are required).
2. The distribution has to be invariant to flow rate.
3. The distribution has to be invariant to polymer viscosity function, as long as it is restricted to a Power Law behaviour.

In any die that meets these requirements, the flow should not have to be corrected by choker bars or flexible lips. A similar analysis has been done by Nguyen and Kamal (1990).

Concerning the flow model, the following assumptions will be used:

- the viscosity dependance on shear rate of the polymer obeys a Power Law relation;
- in each cross section of the die there is steady shear flow;
- the flow is isothermal;
- there is full slip of the side walls of the die, which are the walls perpendicular to the plane in which the material flows, and no slip on the top and bottom walls of the die, that are parallel to the material flow.

Aspects not included in the design are: swelling, orientation, uniformity of strain history, viscous dissipation, multilayer extrusion, melt fracture and deflections of the die itself. So uniformity of deformation history means uniformity of shear deformation history in this analysis.

The dies dealt with are so-called large aspect ratio extrusion dies, as used for sheet extrusion. A die for (hollow) axisymmetric injection moulding products can be designed likewise; the planar die merely has to be ‘folded’ around a cylinder. This, however, implies that the influence of curvature is neglected. Nguyen and Kamal (1990) analysed a cylindrical coat hanger die using a 3-dimensional finite element technique, thus taking curvature into account.

2.2 Determining the die geometry

For a die of exit width \(2b\) and slit height \(h\), the flow rate \(Q\) is given by:

\[
Q = 2bh\bar{v}_s
\]

\(\bar{v}_s\) being the average flow rate over the slit height. The slit height \(h\) is assumed to be known.

A sketch of the distribution system of the die, which will turn out to be shaped like a coat hanger, is given in figure 1. It consists of a deep manifold of low flow resistance, and a narrow slit region of high flow resistance. Assuming that:
• the density of the polymer is constant over the entire die;
• the pressure gradient in the manifold is always perpendicular to the manifold cross section; and
• the flow in the slit region is always in y-direction,
the main relations describing the geometry can be derived.

The flow rate $Q_m$ at any position $z$ in the manifold equals the flow rate at the die exit between $x$ and $x = b$:

$$Q_m(z) = A(z) \bar{v}_m$$
$$= (b - x)h \bar{v}_m$$

(2)

in which $\bar{v}_m$ is the average velocity across the manifold height and $A(x)$ the manifold cross section area at $x$.

Because the pressure gradients (and therefore the flow direction) in manifold and slit region are perpendicular to their respective cross section, uniform exit velocity requires:

$$\frac{\partial p}{\partial y} = \frac{\partial p}{\partial \xi} \frac{d \xi}{dy}$$

(3)

whereas $\xi$ is the coordinate in manifold flow direction, and subscripts $s$ and $m$ denote slit region and manifold respectively (see figure 1).

From plain geometry it can be found that:

$$\frac{d \xi}{dy} = \sqrt{1 + \left(\frac{dx}{dy}\right)^2}$$

(4)

From equations (3) and (4), the slope of the manifold contour line $y(x)$ can be derived as:

$$\frac{dy}{dx} = -\left(\left\{\left(\frac{dx}{dy}\right)_s \right\}^2 \left\{\left(\frac{dx}{dy}\right)_m \right\} - 1\right)^{-\frac{1}{2}}$$

(5)

Equations (2) and (5) determine the shape of the die. To complete the design, one additional condition out of the following three has to be implemented:

i) constant slope of manifold ($\frac{dy}{dx}$ is constant);

ii) uniform shear rate at manifold and slit region walls; or

iii) uniform average residence time.

Although condition iii is actually the one we would like to be met, the second condition will be used for further analysis. It will be shown that, under some additional restrictions, both the second and the third condition will be satisfied. Including only the second condition a priori will make the analysis easier.

The manifold cross section can either be rectangular or circular. The circular manifold turns out to have the following disadvantages over the rectangular manifold:

• the manifold geometry (i.e. contour line $y(x)$) depends on the power law exponent; and
uniform wall shear rate and uniform residence time cannot be achieved together. Moreover, a circular manifold turns out to be curved in three directions, making it almost impossible to manufacture such a die. Thus the analysis will be limited to a rectangular manifold.

Introducing the power law viscosity model;

\[ \eta = \eta_0 \left| \frac{\dot{\gamma}}{\dot{\gamma}_0} \right|^{n-1} \]  

(6)

in which \( \eta_0 \), \( \dot{\gamma}_0 \) denote reference viscosity and reference shear rate, and \( n \) denotes power law exponent, the pressure gradient and wall shear rate can be derived through two-fold integration of the momentum equation for Stokes flow:

\[ \frac{dp}{d\chi} = \eta \frac{\partial^2 v}{\partial z^2} \]  

(7)

This yields:

• for the rectangular manifold \((\chi = \xi)\):

\[ \left( \frac{dp}{d\xi} \right)_m = -\frac{2\eta_0 \dot{\gamma}_0}{h} \left| \frac{\dot{\gamma}_{w,m}}{f_p \dot{\gamma}_0} \right|^n \]  

\[ \dot{\gamma}_{w,m} = -\left( \frac{1}{n} + 2 \right) \frac{2\bar{v}_m}{H} \]  

(8)

(9)

• for the slit region \((\chi = y)\):

\[ \left( \frac{dp}{dy} \right)_s = -\frac{2\eta_0 \dot{\gamma}_0}{h} \left| \frac{\dot{\gamma}_{w,s}}{\dot{\gamma}_0} \right|^n \]  

\[ \dot{\gamma}_w = -\left( \frac{1}{n} + 2 \right) \frac{2\bar{v}_s}{h} \]  

(10)

(11)

whereas \( \bar{v} \) is the average flow rate over the manifold or slit height, \( f_p \) denotes the shape factor, and \( \dot{\gamma}_w \) the wall shear rate. The shape factor corrects for a small \( W/H \) ratio of the rectangular manifold cross section and depends on the power law exponent. Values for \( f_p \) are given by (Tadmor and Gogos, 1979):

\[ f_p = 1 - \frac{192H}{\pi^5 W} \sum_{i=1,3,5,\ldots}^{\infty} \frac{1}{i^6 \tanh \left( \frac{i\pi W}{2H} \right)} \]  

(12)

This relationship has been plotted in figure 2; however, \( f_p \) is assumed to equal 1 for \( W/H > 10 \). For the rectangular manifold, the ratio of pressure gradients in manifold (equation 8) and slit region (equation 10) is independent of viscosity function if:

\[ \dot{\gamma}_{w,s} = \frac{\dot{\gamma}_{w,m}}{f_p} \]  

(13)

From equations (2), (9) and (11) the manifold depth \( H(x) \) can be expressed as:

\[ H(x) = h \sqrt{\frac{b - x}{f_p(x)W(x)}} \]  

(14)
Substituting equations (8) and (10) in (5), the manifold slope turns out to be:

\[ \frac{dy}{dx} = - \left( \frac{b - x}{f_p(x)W(x) - 1} \right)^{\frac{1}{2}} \]  

(15)

At this point two possibilities are left: a manifold of constant width or of constant aspect ratio \( a = W/H \).

**Manifold of constant width**

\[ H(x) = h \sqrt{\frac{b - x}{f_p(x)W}} \quad \text{for} \quad (b - W) \leq x \leq b - W \]  

(16)

\[ y(x) = 2W \sqrt{\frac{b - x}{W}} - 1 \quad ; \quad f_p = 1 \]  

(17)

This is governed by the dimensionless parameter \( D = W/b \).

**Manifold of constant aspect ratio**

\[ H(x) = h \left( \frac{b - x}{af_p h} \right)^{\frac{1}{2}} \]  

(18)

\[ W(x) = aH(x) \]  

(19)

\[ y(x) = \frac{3Bb}{2} \left[ \frac{\sqrt{1 + g(x)}}{g(x)} - \frac{1}{2} \ln \left( \frac{\sqrt{1 + g(x)} - 1}{\sqrt{1 + g(x)} + 1} \right) \right] \quad \text{for} \quad \frac{x}{b} \leq 1 - B \]  

(20)

\[ g(x) = \left[ \left( \frac{H(x)}{h} \right)^{2} - 1 \right]^{-1} \]  

(21)

whereas \( H(x) = h \) at \( y = 0 \).

This case is governed by the dimensionless parameter \( B = \frac{ahf_p}{b} = \frac{Wf_p h}{bb} \).

Uniform average residence time will be obtained if:

\[ \Delta t = \frac{dy}{\bar{v}_s} = \frac{d\xi}{\bar{v}_m} \]  

(22)

Thus, using equations (3), (8), (10) and (13) we obtain:

\[ \frac{d\xi}{dy} = \left( \frac{\partial \xi}{\partial y} \right)_s = \left( \frac{\partial \bar{v}_s}{\partial y} \right)_s \]  

(23)

Condition (22) is already fulfilled if condition (13) is met, so for the rectangular manifold the demand for uniform shear rate at the walls of manifold and of slit region — together with the required invariance to \( \eta_0 \) and \( n \) — implies uniform residence time. From equations (23), (2), (9), and (11) it can also be seen that the distribution is invariant to flow rate: increasing the flow rate increases both \( \bar{v}_m \) and \( \bar{v}_s \) proportionally, thus leaving \( \frac{d\xi}{dy} \) unchanged.

An overview of die geometries resulting from this analysis is given in figure 3. It shows that in order to obtain a shorter die, the manifold width has to be decreased and the manifold height has to be increased. Though some suggest otherwise, the manifold contour of a coat hanger die is always curved (Wang, 1991).
Figure 1: Coat hanger die distribution system. (After Winter and Fritz, 1986.)

Figure 2: Shape factor $f_p$ as a function of aspect ratio $W/H$. (After Tadmor and Gogos, 1979.)
Figure 3: Geometries for coat hanger dies of constant manifold width (left) and constant manifold aspect ratio (right): manifold contours (above) and heights (below). \( D = \frac{W}{5}, B = \frac{Wf_0h}{5H}. \)
3 Verification of some assumptions on the coat hanger die

In order to check whether an exit flow of uniform shear rate and residence time from a coat hanger die, which is designed according to the analysis by Winter and Fritz, can also be obtained numerically, we will simulate the flow in such a die with the VIp program, based on finite element and finite difference methods. This program neglects pressure gradient and velocity in the height direction of the mould (or die) and thus yields two-dimensional pressure results, and velocities in the two main directions of flow; This is known as the lubrication approximation. Thus in VIp two assumptions, that have been introduced in the theoretical analysis of the coat hanger die, have already been incorporated: namely the negligibility of the full slip condition on the side walls, and of the three-dimensional effect of height decrease from manifold to slit region (since pressure gradient is always perpendicular to manifold or slit cross section).

Therefore, before starting the numerical simulation on a coat hanger die, we want to verify whether these assumptions can be justified. This verification will be done by performing some numerical experiments on a test geometry, which grasps all the important aspects of a coat hanger die. Computations will be carried out on three-dimensional flow (with the standard SEPRAN package) and on the approximated three-dimensional flow (with the VIp program, which is a part of SEPRAN). If these assumptions prove to be correct, the VIp will be suitable for numerical simulation of a coat hanger die.

The test geometry is shown in figure 4; geometrical data are given in table 1. It consists of a rectangular manifold, in which the flow enters, and a slit region. Note that the manifold aspect ratio (i.e. the ratio of manifold width to manifold height) equals 10, at which value no pressure correction factor was needed in the theoretical analysis. The main flow direction in the manifold is perpendicular to the main flow direction in the slit region. The fluid is allowed to leave through both manifold exit and slit region exit. The original step-wise decrease in height from manifold to slit region is replaced by a smoother (linear) decrease to suppress numerical problems, due to the rather coarse mesh that had to be used to avoid excessive memory usage.

![Manifold and slit region diagram](image-url)

Figure 4: Mesh for SEPRAN calculations on test geometry.
Table 1: Geometrical data for coat hanger test geometry.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>manifold length $L$</td>
<td>100 mm</td>
</tr>
<tr>
<td>manifold width $2b$</td>
<td>20 mm</td>
</tr>
<tr>
<td>manifold height $H$</td>
<td>2 mm</td>
</tr>
<tr>
<td>slit region length $l$</td>
<td>20 mm</td>
</tr>
<tr>
<td>slit height $h$</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

3.1 Method of verification

The two assumptions mentioned above can be checked by comparing the results of three problems on the test geometry:

1. a three-dimensional flow in SEPRAN with the no slip condition at the side walls;
2. a three-dimensional flow in SEPRAN with full slip at the side walls;
3. an approximated three-dimensional flow in VIP.

The boundary conditions for the first problem are:

- **entry:** $u = \frac{4V_{\text{max}}}{H} \left( z - \frac{z^2}{H} \right)$, $v = 0$, $w = 0$ (24)
- slit side walls: $u = 0$, $\frac{\partial u}{\partial n} = 0$, $w = 0$ (25)
- manifold exit: $\frac{\partial u}{\partial n} = 0$, $v = 0$, $w = 0$ (26)
- slit region exit: $u = 0$, $\frac{\partial v}{\partial n} = 0$, $w = 0$ (27)
- lower and upper walls, manifold side walls: $u = v = w = 0$ (28)

The full slip condition, which is in fact a natural boundary condition, has already been imposed on the slit side walls (equation (25)), since there is no side wall effect in the coat hanger die, simply because the coat hanger slit region does not have any side wall! Equation (24) states that the velocity entry profile is parabolic.

For the second problem, the no slip boundary condition on the side walls (which is included in equation (28)) is replaced by:

- manifold side walls: $\frac{\partial u}{\partial n} = 0$, $v = 0$, $w = 0$ (29)

in which $v = 0$ indicates that the wall is impermeable, and $w = 0$ is maintained to suppress velocity in height direction (as is the case in VIP). In VIP, boundary conditions are imposed by defining injection area(s) and ‘edges’ of the mould. This implies that exit boundary conditions cannot be applied: moulds are supposed not to have exits. To overcome this problem, the test geometry is modified by extending the mould at the ‘original’ exit areas, as
Figure 5: Mesh for VIp calculation on test geometry.
is shown in figure 5. Free ‘exit’ flow conditions now do apply at the original exit areas. The three problems mentioned above enable us to separate the two effects that were discussed in the introducing section. Comparison between the results of the first two problems tells us something about the influence of the manifold side walls. The results of the second (fully three-dimensional) and the third (approximated three-dimensional) problem can be used to detect the influence of the transition from manifold to slit region. Computations have been limited to the case of Newtonian flow.

3.2 A criterion for comparison

As uniformity of residence time is essential for coat hanger dies, the residence times of particles in the flow will be used as a criterion for comparison. Both SEPRAN and VIp contain the particle tracking option, but the way it is treated is different. The two SEPRAN test problems are stationary; after the steady flow has been calculated, a number of user-appointed particles at the entrance are followed ('tracked') until they leave the mesh (Segal, 1993: section PG 9.16). This yields an array of position coordinates at several points in time for each particle, from which the particle track can be reconstructed and residence time can be found. Thus particle tracking is an initial value problem in SEPRAN.

VIp is designed to simulate polymer processing, of which the filling of a mould is the first stage. Since mould filling is instationary in itself, VIp treats the third problem mentioned above as an instationary problem. Particles entering the mould at the injection area are given a label (consisting of injection time or coordinate(s)), which is convected into the mould. Particle tracking in VIp thus is a matter of solving the convection equation (Zoetelief, 1992):

\[
\frac{\partial \xi}{\partial t} = -\xi \vec{V} \cdot \vec{v}
\]

This equation is solved for every filled nodal point; consequently, the label of the particle at every nodal point is calculated at a number of points in time. Residence times can be determined by looking at the labels of nodal points at the manifold and slit region exits at a certain point in time (called observation time), and subtracting the injection times (time labels) from this observation time. Coordinate labels can be obtained directly at the nodal points. Thus particle tracking in VIp can be regarded as an end value problem (although in VIp it is not an end value problem in the mathematical sense!): the exit coordinates and times are known (nodal points are chosen by the user), and injection times and coordinates have to be determined. Note that comparison between SEPRAN and VIp is only useful when the flow in the test region has become more or less stationary!

So in SEPRAN the entry coordinates of the particle tracks are known to the user, whereas in VIp the exit coordinates are known beforehand. Because the positions of the nodal points are determined by VIp and are very unlikely to coincide with the exit coordinates of the SEPRAN particles, comparison based on particle tracking seems rather difficult at first sight. However, by multiplying the input velocity field of the SEPRAN problem of particle tracking by a factor \(-1\), the entire solution field is reversed (i.e. multiplied by \(-1\)), thus enabling us to track particles from exit to entry. By making the starting points of these ‘reverse particle tracks’ coincide with the exit nodal points in VIp, comparison has become possible.
3.3 Results on test problems

The parameters for the test problems are chosen as to resemble the flow of a polymer melt in a coat hanger die (table 2). Since $Re \ll 1$, we are dealing with Stokes flow.

Table 2: Parameters for simple 3-D Stokes flow calculation.

<table>
<thead>
<tr>
<th>type of fluid</th>
<th>Newtonian</th>
</tr>
</thead>
<tbody>
<tr>
<td>density $\rho$</td>
<td>$1.0 \times 10^5 \text{ kg.m}^{-3}$</td>
</tr>
<tr>
<td>viscosity $\eta$</td>
<td>$1.0 \times 10^3 \text{ Pa.s}$</td>
</tr>
<tr>
<td>max. velocity $V_{\text{max}}$</td>
<td>$0.01 \text{ m/s}$</td>
</tr>
<tr>
<td>penalty parameter $\epsilon^1$</td>
<td>$1.0 \times 10^{-14}$</td>
</tr>
<tr>
<td>number of elements</td>
<td>$3 \times (10 \times 5 \times 1) = 150$</td>
</tr>
<tr>
<td>type of element</td>
<td>triquadratic brick</td>
</tr>
</tbody>
</table>

3.3.1 Test on side wall effects

Intersections of the three-dimensional velocity fields for the first and second problem as calculated by SEPRAN are shown in figures 6 and 7. Particle tracks are depicted in figure 8 (only for the second problem). Particle tracking results have been summarized in figure 9 and in tables 3 and 4. Note that particle tracking was performed from 'exit' to 'entry'. Looking at figure 9, we notice that the difference in entry $y$-coordinates increases as the particle is flowing closer to the manifold side wall. The same tendency is revealed in the difference between residence times. These differences, as to be expected, are relatively small.

3.3.2 Test on effects of height transition

The results for the third problem (calculated by VIp) can be seen in figures 10, 11, and 9, and in table 5. Some oscillation shows up at the slit region exit, which seems to locally increase the injection time labels, and thereby decrease residence times. To get some idea about the influence of the height transition zone, we have to compare the '*'- and 'o'-marked points in figure 9 (corresponding with tables 4 and 5). Residence times in VIp are generally 2 seconds shorter than in SEPRAN, even for particles that do not pass the transition zone. This may also be due to the difference in particle tracking algorithms between SEPRAN and VIp. Note, however, that $y$-labels (entry $y$-coordinates in the SEPRAN-tables) are remarkably similar.

3.4 Conclusions

Since the influence of side walls on residence time is rather small, the assumption that this effect can be neglected is justified. This also holds for the effect of height transition from manifold to slit region. The discrepancy in residence times between SEPRAN and VIp can partly be accounted for by some numerical oscillation in VIp, and by the difference in particle tracking algorithms.
Figure 6: Intersection at $z = 0.5\text{ mm}$ (above) and at $z = 25\text{ mm}$ (below) of SEPRAN velocity field in test geometry with side wall effects.
Figure 7: Intersection at \( z = 0.5 \text{mm} \) of SEPRAN velocity field in test geometry without side wall effects.

Figure 8: SEPRAN particle tracks from exit to entry in test geometry without side wall effects (time span between two small circles on a track is 2 seconds).
Figure 9: Summary of particle tracking results on SEPRAN test problems with and without side wall effects, and on VIp test problem.
Figure 10: VIP time labels for test geometry.
Figure 11: Vlq y-labels (in midplane) for test geometry.
Table 3: SEPRAN particle tracking results on test geometry with side wall effects

<table>
<thead>
<tr>
<th>Particle number</th>
<th>exit coordinates</th>
<th>entry coordinates</th>
<th>residence time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$x$ [mm]</td>
<td>$y$ [mm]</td>
<td>$x$ [mm]</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
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<td>0</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>8</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>100</td>
<td>12</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
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<tr>
<td>5</td>
<td>80</td>
<td>40</td>
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<td>6</td>
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<td>9</td>
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<td>40</td>
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</tr>
<tr>
<td>11</td>
<td>10</td>
<td>40</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>5</td>
<td>40</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4: SEPRAN particle tracking results on test geometry without side wall effects.

<table>
<thead>
<tr>
<th>Particle number</th>
<th>exit coordinates</th>
<th>entry coordinates</th>
<th>residence time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$x$ [mm]</td>
<td>$y$ [mm]</td>
<td>$x$ [mm]</td>
</tr>
<tr>
<td>1</td>
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<td>0</td>
</tr>
<tr>
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<td>100</td>
<td>12</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
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<td>5</td>
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<td>40</td>
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</tr>
<tr>
<td>7</td>
<td>45</td>
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<tr>
<td>10</td>
<td>20</td>
<td>40</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
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<tr>
<td>12</td>
<td>5</td>
<td>40</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 5: VIp particle tracking results on test geometry without side wall effects

<table>
<thead>
<tr>
<th>Nodal point</th>
<th>exit coordinates</th>
<th>y-label [mm]</th>
<th>residence time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>63</td>
<td>100 4</td>
<td>1.50</td>
<td>18.33</td>
</tr>
<tr>
<td>105</td>
<td>100 8</td>
<td>2.98</td>
<td>18.33</td>
</tr>
<tr>
<td>147</td>
<td>100 12</td>
<td>4.41</td>
<td>18.33</td>
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<tr>
<td>189</td>
<td>100 16</td>
<td>5.69</td>
<td>18.33</td>
</tr>
<tr>
<td>437</td>
<td>80 40</td>
<td>8.42</td>
<td>26.99</td>
</tr>
<tr>
<td>433</td>
<td>60 40</td>
<td>9.56</td>
<td>14.75</td>
</tr>
<tr>
<td>430</td>
<td>45 40</td>
<td>11.24</td>
<td>10.42</td>
</tr>
<tr>
<td>428</td>
<td>35 40</td>
<td>12.79</td>
<td>8.02</td>
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<tr>
<td>426</td>
<td>25 40</td>
<td>14.68</td>
<td>5.54</td>
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<tr>
<td>425</td>
<td>20 40</td>
<td>15.80</td>
<td>4.66</td>
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<td>423</td>
<td>10 40</td>
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<tr>
<td>422</td>
<td>5 40</td>
<td>18.47</td>
<td>2.20</td>
</tr>
</tbody>
</table>
4 Coat hanger die simulations

Both types of coat hanger dies as described in the first section have been analysed using the VIP program. The geometrical and material data were adopted from Winter and Fritz (1986), the coat hanger die with constant manifold width being die I, and the one with constant aspect ratio being die II in their article. The pressure correction factor \( f_p \) for die II is not given explicitly, but can be derived in several ways from the geometrical data. However, this factor cannot be uniquely determined from the data of Winter and Fritz. Therefore, \( f_p = 1 \) has been used in the analyses of both dies. Again, the die mesh is extended in order to obtain some kind of stationary flow in the die itself. Because of its symmetry, only half of the die need to be meshed. A linear transition zone of 1 mm is inserted between manifold to slit to established a linear decrease from manifold to slit region height.

4.1 Coat hanger of constant manifold width

The geometrical data of the coat hanger die of constant manifold width are given in table 6, while the material and computational parameters are summarised in table 7. The entrance flow is based on a mass flow of 25 kg/h (as in Winter and Fritz, 1986) and an assumed mass density of 1000 kg/m\(^3\). The mesh for this type of coat hanger is presented in figure 12. The thick line parallel to the x-axis indicates the actual die exit.

Table 6: Geometrical data for coat hanger die of constant manifold width. (After Winter and Fritz, 1986.)

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>half die width</td>
<td>94.24 mm</td>
</tr>
<tr>
<td>manifold width</td>
<td>20.0 mm</td>
</tr>
<tr>
<td>initial manifold height</td>
<td>3.91 mm</td>
</tr>
<tr>
<td>slit height</td>
<td>1.8 mm</td>
</tr>
<tr>
<td>maximum slit length</td>
<td>77.1 mm</td>
</tr>
</tbody>
</table>

Table 7: Material and computational parameters for coat hanger die simulation.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>type of fluid</td>
<td>Power Law</td>
</tr>
<tr>
<td>zero viscosity</td>
<td>( \eta_0 )</td>
</tr>
<tr>
<td>Power Law exponent</td>
<td>( n )</td>
</tr>
<tr>
<td>entrance flow</td>
<td>( Q )</td>
</tr>
<tr>
<td>density</td>
<td>( \rho )</td>
</tr>
<tr>
<td>number of elements</td>
<td>430</td>
</tr>
<tr>
<td>number of grid points</td>
<td>9</td>
</tr>
</tbody>
</table>

Figure 13 shows that the pressure distribution is reasonably well in accordance with the assumption by Winter and Fritz, that the pressure gradient should be along the main flow direction. Also the flow behaves accordingly. Because of the 'artificially' stationary flow in the die region, the x-label lines in the slit region also represent stream lines (figure 14). The
essential point of the coat hanger die is to obtain a uniform residence time over the entire die exit. Particles that have been injected at the same time are supposed to leave through the exit at the same time. Therefore we have to check the injection time labels in figure 14. We see that the results from VIP do not entirely match with the concept of uniform residence time in three respects:

1. The particle leaving at the outer side of the exit (at \( z \approx b \)) appear to have a longer residence time than the particles leaving from the slit region or from the inner side of the manifold. This is due to the flow path being longer at the outer side of the manifold than at the inner side. This effect has not been covered in the theoretical analysis. It has already been partly compensated for by having the injection area parallel to the die exit, instead of perpendicular to the manifold, which elongates the flow path of particles moving along the inner side of the manifold.

2. Some kind of deviation shows up at the symmetry axis of the die; it is believed to be caused by the sharp angle between this axis and the inner contour line of the manifold.

3. The lines of equal injection time labels are somewhat curved in the slit region. This is probably caused by the two effects mentioned above.

In spite of these deviations, the residence time is still quite uniform over the exit, especially in the slit region. These results might be improved by slightly decreasing the manifold height towards the outer manifold wall. This, however, has not been checked.

A final check can be done by comparing the wall shear rate results with the theoretical prediction (wall shear rate is supposed to be uniform). Figure 15 shows that the shear rate is quite uniform over the die. The wall shear rate can be calculated from equations (1) and (11); its value is \( 215 \, \text{s}^{-1} \). VIP yields a wall shear rate of about \( 220 \, \text{s}^{-1} \) which is close enough. Both flow rate and power law exponent were changed to check whether the uniformity of residence time is invariant to these parameters. A change in flow rate did indeed give similar results. The injection time label and wall shear rate distributions for a power law exponent \( n \) of 0.7 (leaving the other parameters unchanged) are given in figure 16; these are also similar to the results on \( n = 0.4 \). Wall shear rates from theoretical analysis and VIP are 164 \( \text{s}^{-1} \) and 175 \( \text{s}^{-1} \) respectively.

### 4.2 Coat hanger of constant manifold aspect ratio

For the coat hanger of constant aspect ratio, the data on geometry are given in table 8. The mesh for this coat hanger die can be seen in figure 17. Material and computational parameters have not been changed.

The results for this coat hanger die can be seen in figures 18 to 20. Concerning the uniformity of residence time, the same remarks that were made on the coat hanger die of constant manifold width apply here. However, the influence of the manifold itself is smaller, since the difference in flow path lengths within the manifold is considerably less. Furthermore, wall shear rate is almost perfectly uniform and within 3% to the value predicted from analysis.
Table 8: Geometrical data for coat hanger die of constant manifold aspect ratio. (Based on Winter and Fritz, 1986.)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>half die width</td>
<td>$b$</td>
</tr>
<tr>
<td>manifold aspect ratio</td>
<td>$a$</td>
</tr>
<tr>
<td>initial manifold height</td>
<td>$H$</td>
</tr>
<tr>
<td>slit height</td>
<td>$h$</td>
</tr>
<tr>
<td>maximum slit length</td>
<td>$l$</td>
</tr>
</tbody>
</table>

Figure 12: Mesh for coat hanger die of constant manifold width.
Figure 13: Coat hanger die of constant manifold width \((n = 0.4)\): height \((above)\) and pressure distribution \((below)\).
Figure 14: Coat hanger die of constant manifold width ($n = 0.4$): injection time (above) and $x$-labels (below) in midplane.
Shear rate

Min, Max: $0.000E+00$ $5.850E+02$ [1/s]

Figure 15: Coat hanger die of constant manifold width ($n = 0.4$): wall shear rate distribution.
Figure 16: Coat hanger die of constant manifold width ($n = 0.7$): midplane injection time labels (above) and wall shear rate distribution (below).
Figure 17: Mesh for coat hanger die of constant manifold aspect ratio.
Figure 18: Coat hanger die of constant manifold aspect ratio \( (n = 0.4) \): height (above) and pressure distribution (below).
Figure 19: Coat hanger die of constant manifold aspect ratio ($n = 0.4$): injection time (above) and $x$-label (below) in midplane.
Figure 20: Coat hanger die of constant manifold aspect ratio ($n = 0.4$): wall shear rate distribution.
5 Conclusion

A die that produces a flow with uniform residence time, uniform wall shear rate and uniform average exit velocity for a Power Law fluid can be achieved by using a specific die geometry, the so-called coat hanger die, which is obtained from theoretical analysis. Since the influence of side walls and transition from manifold to slit region is rather small, the flow in a coat hanger can be simulated with the VIp package. Global tendencies seem to be correct.

Numerical simulation has been carried out for two types of coat hanger dies with the VIp program. The results match well with the theoretical analysis by Winter and Fritz. Uniform residence time, uniform wall shear rate and uniform average exit velocity are indeed invariant to flow rate and Power Law exponent. Uniformity of residence time cannot be obtained completely, due to some simplifications in the theoretical analysis and geometrical irregularities. The prospect of having a polymer flow coming out of the die with a uniform residence time distribution is very promising when dealing with the reaction injection moulding process (RIM). The uniform residence time ensures uniform conversion of the material entering the mould, provided the temperature has been uniform over the die walls. With the VIp program, numerical simulation of a RIM process in which the mould is attached to a coat hanger die should be possible.
References


