6. Application of the finite volume method to the planar 4:1 contraction

In chapter 5 the finite volume/finite difference algorithm has been described so solve the UCM-model. In this chapter this numerical treatment is applied to the abrupt planar 4:1 contraction problem.

In section 6.1 the test problem with its geometrical parameters is described, while in section 6.2 the numerical and physical parameters are given. This section also presents the results obtained by this algorithm. The stretching of the salient corner vortex to the re-entrant corner with increasing Deborah numbers will be shown. And the change from a concave vortex to a convex vortex will be demonstrated. At a Deborah number of \( \approx 11 \) the calculations will be stopped, since at this Deborah number the tensor \( \tau_A \) will become indefinite and the desired convergence criterion will not be satisfied. Since \( \tau_A \) contains a negative eigenvalue the analytical problem has become ill-posed. Also the convergence criterion for a steady state solution was not met, but since the analytical problem becomes ill-posed if \( \tau_A \) becomes indefinite, it is not sure whether the flow becomes time dependent or the lack of convergence should be attributed to the lack of well-posedness.

Section 6.3 gives an overview of the performance of this numerical method when applied to the abrupt planar 4:1 contraction.

6.1 Test problem: the planar 4:1 contraction

One of the most challenging test problems is the flow through an abrupt 4:1 contraction, either the planar or the axisymmetric contraction, both from the analytical, numerical and experimental point of view. Especially the development of the corner vortex, the appearance of a lip vortex and the enormous growth, in the case of the axisymmetric contraction, of the corner vortex in the flow of polymer melts and solutions has been a subject of study the last 20 years. Beautiful experimental work has been performed and reported by McKingley et al. [40] and Evans and Walters [22], [23].

The geometry of the planar 4:1 contraction consists of two channels, the inflow channel of width \( D_u \) and the outflow channel of width \( D_d \), where \( D_u > D_d \). The ratio \( D_u : D_d \) is called the contraction ratio. In the following the contraction ratio \( D_u : D_d \) will be 4:1. At the point where these two channels meet a sudden contaction of inflow channel into the outflow channel takes place. The length of the upstream channel is given by \( L_u \) and the length of the downstream channel by \( L_d \). This geometry is depicted in Fig 6.1.

Numerical solutions for this type of flow are very hard to obtain due to the presence of the singularity of the velocity gradient at the re-entrant corner. The finite element
method developed by Marchal and Crochet [39] was able to reach a stationary solution, by means of a stationary algorithm, beyond $De = 20$, although the tensor $\tau_A$ lost positive definiteness at $De = 7$, in which $De = \lambda \dot{\gamma}_w$, where $\lambda$ is the relaxation time and $\dot{\gamma}_w$ is the shear rate along the downstream wall for the fully developed flow.

Time dependent calculations $We = 2$, Carew et al. [16] were restricted to $We = 2$, for the Oldroyd-B model, although there solution at $We = 1$ is fraught with wiggles in the normal stress difference and the shear stress upstream of the contraction. For the PTT model they were able to reach $We = 15$, with $\epsilon = 0.02$. In a later paper by these authors [17] performed a calculation at $We = 5$ for the Oldroyd-B model by means of incorporating a shock capturing mechanism into their numerical scheme. The results show large irregularities downstream the contraction and no steady state was reached.

The length of the downstream channel is denoted by $L_d$ and the length of the upstream channel by $L_u$.

### 6.2 Numerical results for the 4:1 contraction

The 4:1 test problem is solved with the numerical method described in the previous chapter. The parameters used are: $L_u = L_d = 50$, $D_u = 8$, $D_d = 2$. The grid used consists of 800 cells in the $x$-direction and 32 cells in the $y$ direction, so $dx = dy = 0.125$. The time step used is $\Delta t = 0.005$. All the solutions presented in this section have converged in the sense that $\max_{i,j} \| (\phi^{n+1} - \phi^n) / \Delta t \| \leq 10^{-12}$, in which $\phi$ is either $u$, $v$, $\tau_{11}$, $\tau_{22}$ or $\tau_{12}$.

The only parameter which is changed in the following examples is the relaxation time $\lambda$, while the inflow velocities are kept the same. The Deborah number in all calculations is defined by $De = \lambda \dot{\gamma}$, in which $\dot{\gamma}$ is the shear rate at the wall of the downstream channel.
The specific mass \( \rho = 1 \) and the viscosity \( \eta = 1 \) throughout, so the Reynolds number is approximately \( Re = 0.5 \).

6.2.1 The re-entrant corner

In the summary at the end of chapter 1 it was remarked that many numerical models perform well in smooth geometries, but problems arise near geometrical discontinuities such as for example a re-entrant corner.

Several authors have tried to describe the flow and stresses near a sharp corner analytically. For instance Hinch [26] and Davies and Devlin [19] give expressions for the stream function and the extra-stress components in the vicinity of the corner, using asymptotic methods. These authors come to the conclusion that the stresses in the vicinity of the corner behave like \( r^{-\alpha} \), in which \( \alpha \) is a positive constant, preferably less than unity in order that the stress solution is integrable near the corner.

Also from the numerical point of view much attention has been focused on the behaviour of the flow near the re-entrant corner. In Renardy [50] both the problem is addressed from the analytical and the numerical point of view. The most interesting part of this paper is that the large normal stress peaks downstream from the corner, which are usually encountered in numerical simulations of viscoelastic fluids in contraction flows, disappear if the grid is refined. For very fine grids the extrema in the normal stress component finally disappears. The only drawback is that these calculations are based on a given Newtonian velocity field, so the interactions between the momentum- and constitutive equations is lost.

The staggering of the unknowns employed in this work circumvents the evaluation of the normal stresses at the corner itself, but one still has to calculate the shear stress at the corner. Since the velocity gradient is discontinuous at that point it is impossible to assign a definite value to the shear stress value at the corner. Furthermore, in order to solve the differential equation at the re-entrant corner one has to have the normal stress components at the corner and these variables are also ill-defined. This problem may be circumvented by treating the shear stress value at the corner as an interior point. This means that the normal stress values are interpolated from its three nearest cells. Also the extension rates \( u_x \) and \( v_y \) are interpolated from these three cells.

Obviously the normal stress values and shear stress values at the corner, defined thus, do not coincide with the real value of these extra-stress components at the corner, since these values are not well defined. Since the finite volume method is a weighted residual method in which the stress components represent the average value in the cell and not the value in the collocation point itself one may hope that these approximations give a fairly good approximation of the stresses in the neighbourhood of the re-entrant corner.

6.2.2 Numerical results for various values of \( De \)

In this section the solution for several values of the Deborah number are investigated. For very small Deborah numbers the flow pattern is the same as the flow for the Navier Stokes solution. At a Deborah number of approximately 4.5 the salient corner vortex extents...
to the re-entrant corner. Above a Deborah number of 10 the form of the vortex changes from concave to a convex vortex.

The sign of the determinant $\mathbf{\tau}_A$ is evaluated both in the center of the cells and at the vertices of the cells. The numerical calculations show that up to $De = 4$ the determinant of $\mathbf{\tau}_A$ is ultimately bounded from below by $(\eta/\lambda)^2$ even when this was not the case initially. This means that $\det \mathbf{\tau}_A$ grows in time as is to be expected from the analysis presented in section 3.8. For Deborah numbers exceeding 4 this lower bound is not satisfied by the stress tensor evaluated at the re-entrant corner, although the determinant is still positive. In the last calculation presented $\det \mathbf{\tau}_A$ has become negative in several points surrounding the re-entrant corner and the convergence criterion has not been met. Either the flow has become time-dependent, i.e. $\partial \phi / \partial t \neq 0$ or the ill-posedness of the system, due to $\det \mathbf{\tau}_A < 0$ prevents the scheme from convergence.

Finally the MCSH approach is tested by using different values of $N$ in the approximation of the exponential series, Eq. (5.13). It turns out that for low values of $N$, $N = 1, 2$ the determinant of $\mathbf{\tau}_A$ becomes negative for moderate Deborah numbers, whereas when the approximation described in the previous chapter is used the system of equations remains well-posed until $De = 10$.

Fig. 6.2 shows the streamlines near the re-entrant for $De = 0.75$. In this calculation the determinant of $\mathbf{\tau}_A$ is ultimately larger than $(\eta/\lambda)^2$, the lower bound which was derived in chapter 3. The stress components along the line $y = 3$ are given in Fig 6.3. Note that a stress peak for the $\tau_{11}$ component is absent. In many numerical calculations this component possesses a large peak which may increase in time for the Upper Convected Maxwell model. In the aforementioned paper by Renardy [51] it is argued that this peak in the $\tau_{11}$ stress component is a numerical artifact. Since there are no normal stress components defined at the corner no problems are encountered for these values. These calculations show that no peak in the $\tau_{11}$ is present.

If the Deborah number is increased from 0.75 to 1.5 the vortex remains the same. The isolines for the extra-stress components are given in Fig. 6.4. These plots reveal that stress boundary layers develop downstream of the re-entrant corner, but no wiggles or any other lack of smoothness is encountered. The stresses along the line $y = 3$ for $De = 1.5$ are

Figure 6.2: Streamlines near the re-entrant corner, $De = 0.75$. 
The $t_{11}$ stress component along the line $y=3$

Figure 6.3: *The extra-stress components along the line $y = 3$ for $De = 0.75$.*

The $t_{22}$ stress component along the line $y=3$

Figure 6.4: *The isolines of the $\tau_{11}$, $\tau_{22}$ and shear stress component resp. at $De = 1.5$.*

given in Fig. 6.5. Compared to the stresses along the line $y = 3$ for $De = 0.75$, the $\tau_{12}$ and $\tau_{22}$ plots are almost identical, although the peak in the shear stress is slightly higher for $De = 1.5$. A significant change in values of the $\tau_{11}$ along the line $y = 3$ is observed, especially in the level of the normal stress component in the downstream channel. Again, there is no stress peak in the $\tau_{11}$ component along the line $y = 3$. The peaks in the shear stress and the $\tau_{22}$ component are stable, in the sense that they do not grow in time.

In both calculations the determinant of $\mathbf{T}_A$ was ultimately bounded from below by $(\eta/\lambda)^2$, which again confirms the analysis in section 3.8. The velocity components along the line $y = 3$ are given in Fig. 6.6. Fig. 6.7 shows that increasing the Deborah number further to
Figure 6.6: The $x$- and the $y$-component of the velocity along the line $y = 3$ for $De = 1.5$.

Figure 6.7: Streamline plot in the neighbourhood of the re-entrant corner for $De = 3$ and $De = 4.5$, resp.

3 and 4.5 does not significantly change the shape and the intensity of the corner vortex. Again, the determinant of $\mathbf{r}_A$ satisfies the lower bound condition mentioned above, except the determinant at the re-entrant corner. However, in the step from $De = 4.5$ to $De = 6$ this condition is violated at points in the neighbourhood of the re-entrant corner, although the tensor remains positive definite. Moreover, the shape and intensity of the corner vortex changes significantly as can be seen in Fig. 6.9. Carew et al. [16] witnessed this change of the flow pattern for $We \approx 15$, $We = \lambda U/L$, but only with the PTT model, $\epsilon = 0.02$. In Baloch et al. [9] stream plots are shown for the PTT model for various values of $\epsilon$, ranging from $\epsilon = 0.25$ to $\epsilon = 0.02$. These plots show that the size of the vortex increases with decreasing $\epsilon$. In the limit $\epsilon \to 0$, their model reduces to the Oldroyd-B model. Unfortunately, this group was unable to increase the Weissenberg number from $We = 1$ to $We = 2$ for the Oldroyd-B model, so no comparison with the case $\epsilon = 0$ can be performed, but one expects that in that case the increase of the vortex should appear at an even lower value of the Weissenberg number. Furthermore, since the Maxwell model is more elastic than the Oldroyd-B model, the sudden growth of the vortex seems reasonable for $De \approx 4.5$.

The stretching of the vortex from the salient corner to the re-entrant corner has also been observed in experiments by Boger et al. [13] and Evans and Walters [22],[23]. However, the dynamics of the flow as a function of the Deborah number depends also critically on the fluid inertia, contraction ratio and the rheological properties of the fluids. One
scenario is that at a certain Deborah number apart from the vortex in the salient corner a small vortex near the re-entrant corner develops, the so-called lip-vortex. Both the intensity of this lip-vortex and the salient corner vortex increase with the Deborah number and finally the corner vortex coalesces with the lip vortex. This situation is present in Fig. 6.9 in which both the salient corner vortex and the lip-vortex are present, both engulfed in an enveloping vortex. In this series of calculations no separate lip vortex was encountered for the steady state solution, instead the salient corner vortex stretching along the contraction to form larger vortex. If the Deborah number is increased from $De = 4.5$ to $De = 5$ a single lip vortex is temporarily present. Fig 6.8 shows the steady state solution for $De = 4.76$ where the vortex just leaves the salient corner vortex. Both vortices are contained in a larger enveloping vortex, but the small vortex just beneath the re-entrant corner is clearly visible. After $De = 7.5$ the vortex changes form, from a concave to a convex vortex. An example of such a convex vortex is given in Fig 6.10. No attempts have been made to increase the Deborah number even higher since the tensor $\mathbf{\tau}_A$ lost positive definiteness for a Deborah of approximately 10. Furthermore the convergence requirement, $\|\phi^{n+1} - \phi^n\| \leq 10^{-12}$ could not be attained, but $\|\phi^{n+1} - \phi^n\| \approx 10^{-7}$. However no divergence occurred. Since the (analytical) problem becomes ill-posed it is hard to judge whether this is the onset of
time-dependent behaviour.

In chapter 4 it was mentioned that several papers described that in the transient phase, after the Deborah number was instantaneously increased a lip vortex appeared which slid down the wall and finally is swallowed by the salient corner vortex. This phenomenon was present in all the calculations reported here, even in the case where the vortex nearly reaches the re-entrant corner. In this case a lip vortex appeared with high vorticity. The vortex slides down the wall, while the vorticity decreased.

Another feature of viscoelastic flows in a contraction is the overshoot of the velocity along the centerline. This overshoot is more pronounced for higher Deborah numbers. Fig. 6.11 shows the velocity overshoot for various Deborah numbers.

Figure 6.10: For $De = 11.03$ the a convex vortex appears

Figure 6.11: Velocity overshoot along the centerline for the Deborah numbers $De = 1.5$, $De = 3$, $De = 4.5$, $De = 6$ and $De = 7.5$. The highest Deborah number displays the highest overshoot.

As was mentioned in this chapter the ultimate steady state solution depends on the time step used. However, solutions obtained by different time steps are almost identical and so is the transient solution to the steady state.

More dramatically the solution changes if in the exponential operator only a limited number of terms is evaluated. For $N = 1$, which is equal to setting $F = I + \Delta tL$, the determinant of $\tau_A$ becomes indefinite at $De \approx 4$, indicating that the analytical solution would be Hadamard unstable in that particular point. Only if a sufficient number of terms is used in the approximation of the deformation gradient the tensor $\tau_A$ remains positive
definite for at least up to $De = 10$ for all points excluding the stresses at the re-entrant corner.

These calculations have also been performed on a $400 \times 16$ grid and the converged solutions have been obtained up to $De = 9.5$ after which the tensor $\tau_A$ became indefinite and the convergence criterion could not be attained. The spatial resolution of these calculations is poor compared to the results shown in this chapter. The calculations on the refined mesh however suggest that the attainable Weissenberg number increases with mesh refinement in contrast to the phenomenon described in chapter 4 where it was noted that for some algorithms the attainable Weissenberg number decreased with mesh refinement. Unfortunately no results of calculations on a $1600 \times 64$ grid can be presented since for this size the algorithm becomes very slow and no attempt has been made to solve the equations on this mesh.

Although the algorithm seems to give good results for Deborah numbers slightly over 10, the tensor $\tau_A$ does not satisfy the lower bound for the derivative and eventually becomes indefinite. There might be two reasons why the algorithm finally breaks down.

- The determinant of $\tau_A$ is convected along the streamlines analytically. If this determinant is positive initially and a monotone scheme is used to approximate the convection along the streamlines, this determinant remains positive. First order upwinding is a monotone scheme so the determinant should remain positive, however since it is not possible to cancel out the terms $\partial v/\partial x$ in the $\tau_{22}$-equation and the $\tau_{12}$-equation and the term $\partial u/\partial y$ in the $\tau_{11}$- and $\tau_{12}$-equation, the analysis given in chapter 3 is not applicable to the discrete system. Especially in regions where the shear rates are large and/or where the shear rates change dramatically the two different approximations in the normal stress equations and the shear stress equation may lead to large error in the determinant of $\tau_A$.

- Even if the characteristic equation along the streamlines could be extracted discretely from the set of algebraic equation, the elliptic operator in the wave equation will in general have complex eigenvalues, since the tensor $\tau_A$ appearing in this operator will in general not be symmetric. If the imaginary part of these eigenvalues becomes too large with respect to the damping term $\tau/\lambda$ in the constitutive equation the system becomes Hadamard unstable and artificial velocity gradients may appear.

Further research has to determine which of the above mentioned causes leads to the limits on the attainable Weissenberg number.

### 6.3 Summary

In this chapter the numerical scheme developed in chapter 5 has been applied to the planar 4:1 abrupt contraction. Converged solutions have been given for Deborah numbers exceeding 11. No further increments of the Deborah number have been tried, since for $De = 11$ the tensor $\tau_A$ became indefinite in many points in the neighbourhood of the re-entrant corner. The lower bound (see section 3.8) on the determinant of $\tau_A$ was violated already at $De \approx 6$ in the vicinity of the re-entrant corner.
This method yields smooth velocity and stress fields throughout the computational domain. Particularly the stress peak in the $\tau_{11}$ variable at the re-entrant corner which is present in many numerical calculations is absent since this variable is not evaluated at the re-entrant corner. The development of the salient corner vortex to the re-entrant corner has been captured for $De \approx 4.5$. No isolated lip vortex has been found, but experiments show that this need not be the case.

In chapter 2 it has been mentioned that using the MCSH-history approach leads to a steady state solution which is still dependent on the time step $\Delta t$. Application of the above algorithm has shown that the solutions are indistinguishable when obtained with different time steps. The differences for different approximations of the deformation gradient on the other hand are very significant. If in the series approximation of the exponential operator only 2 terms are evaluated the tensor $\tau_A$ becomes indefinite at $De \approx 4$ and the lower bound on the determinant of this tensor is only satisfied up to $De \approx 2$. Increasing the number of terms in the approximation of the exponential operator leads to a more stable time integration. The accuracy of the approximation given by Eq. (5.13) approximates $\exp(\text{tr} L)$ up to machine accuracy. The value of $N$ to reach this accuracy is almost everywhere equal to 1, except near the re-entrant corner where more terms have to be evaluated in order to achieve the desired accuracy.

Finally at $De > 11$ the tensor becomes indefinite in a region around the re-entrant corner. This may be due to the fact that the hyperbolic part along the streamlines cannot be extracted discretely from the set of algebraic equations since the shear rate in the normal stress equations and the shear rate equation are defined differently. This hyperbolic part describes the convection of $\det \tau_A$ through the computational domain. If first order upwinding is applied to this hyperbolic part the determinant will remain positive. Furthermore, a staggered grid is not suitable to obtain a symmetric elliptic operator which appears in the wave part of the hyperbolic part. The presence of complex eigenvalues in $\tau_A$, appearing in this operator may lead to artificial gradients, which in turn enter into the convection part along the streamlines, causing the determinant of $\tau_A$ to become indefinite.

Although some deficiencies are attributed to the use of the staggering, which may lead to the indefiniteness of the tensor $\tau_A$, the test problem does not possess a unique solution at the re-entrant corner, which may also be the cause of breakdown of the algorithm. Further investigations, in which the sharp re-entrant corner is replaced by a rounded corner, have to clarify whether this is the source of trouble.