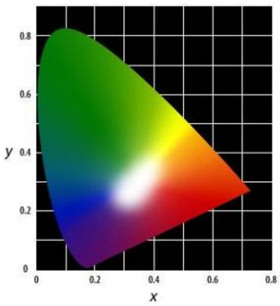
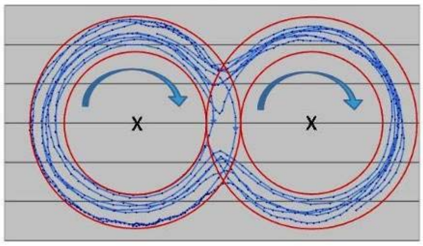
Machine Design Handbook





The PEPT-Flow project is supported by funding under the Sixth Framework Programme of the European Union.

Contract No. COLL-CT-2006-030191.

Table of Content

1 Twin Screw extruders – basic principal

1.1 Introduction

The compounding of thermoplastic materials on an industrial scale is mainly carried out in co-rotational twin-screw extruders (TSE) that were specifically designed to offer high-throughput and good mixing capabilities. Due to the inherent flexibility in the machine design of TSEs, where barrel segments, screw elements and dosing points can be varied, it is possible to adapt this machine to the manufacturing of a large variety of thermoplastic compounds. Typical adaptations are the use of modified screw profiles tailoring the amount of mechanical mixing, residence time and pressure levels, within limits, to specific needs of the material system.

1.2 General machine concept

A twin-screw extruder is a machine with two single screws. There are a tremendous variety of twin-screw extruders, with differences in design, principle of operation, and field of applications.

Twin-screw extrusion is a very flexible process. This flexibility is mainly due to a modular design of both the screw and the barrel (see figure 1-2-1). The screw can be configured in a number of different ways, enabling the degree of mixing and conveying to be controlled.

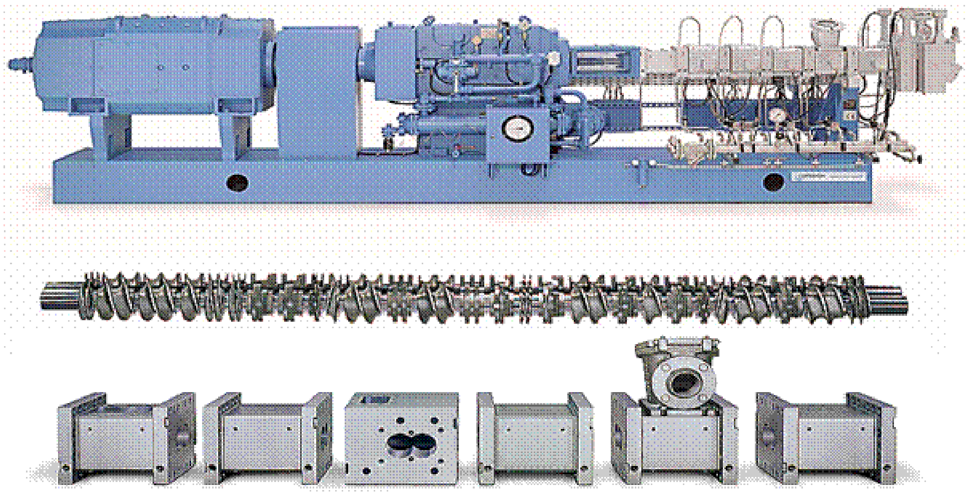


Figure 1-2-1: Machine concept of twin-screw extruder

Not only can the screw and barrel be configured differently, but material can be fed into the extruder in a number of ways. The extruder is fitted with a hopper for the main feed.

For the dosing of fillers, fibres, additives and additional polymers to be blended, a second or third feed port can be fitted to the extruder downstream of the material flow. This feeding is mainly done by so called side-feeder, squeezing the material into the already molten polymer material.

For the dosing of liquids injection nozzles can be fitted in different positions, typically in areas with low melt pressure.

For the stripping of unwanted low-molecular weight volatiles several venting options are possible. Atmospheric venting allows removal of these components at atmospheric pressure, being effective for volatiles with low boiling point. Vacuum degassing is far more effective in the removal of low molecular components. Several technical options have been developed in the past to allow effective degassing under very different operating conditions, including special side-feeder type degassing devices that allow the degassing of compounds that show a lot of foaming.

Combining these very different processing options, TSE's offer a very broad flexibility that allows the processing of very different material systems on the same base machine. On the other hand this flexibility can only lead to economic and competitive compounding, if at least most of the options and configuration possibilities are being used to reach optimum material properties at the highest possible machine outputs.

The following figure graphically illustrates the flexibility of modern compounding processes including different options for pelletizing.

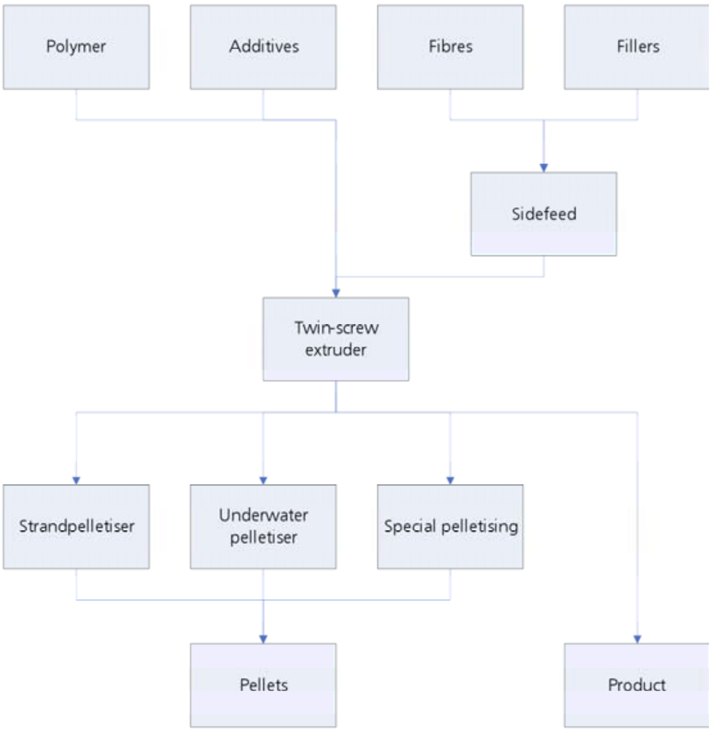


Figure 1-2-2: TSE feeding and pelletizing options.

The characteristics of a TSE can be described in the following summary:

- Twin screws are very efficient at conveying and mixing
- Mixing and the composition of thermoplastic compounds can be controlled by machine configuration.
- TSE are mainly Starve Fed to prevent them reaching their Torque limit

- Throughput is Independent of Screw Speed
- Gravimetric or Loss in weight (LIW) feeders are used to monitor flow to the hopper
- More than one feeder can be used thus enabling accurate continuous blending
- Configuration is vital for reaching economically and technically optimised compounding.

1.3 Flexibility in Process design

As already described in the introduction, co-rotating twin-screw extruders are often designed and manufactured in a segmented/modular construction. This practice not only avoids the need to hold tight bore tolerances over a long barrel length but also aids screw change and cleaning, it furthermore offers flexibility to adapt machines to different material compounding needs.

TSE screws are made up of individual sections that slide onto a keyed or splined shaft. [The assembly contains not only forward pumping right-handed helical screw elements, but also special mixing elements, which can exert a pumping action.]? Left-handed screw elements, which pump backwards, are also found.

The modular approach also applies to the barrel sections. Barrel sections with feeding ports or vents can be placed along the barrel length. The barrel can differ in length as a different number of sections and lengths of barrel & screw shaft can be used. The length divided by the diameter (L/D) is a convenient method of describing the geometry of the screw and the length is often quoted as the number of diameters. So for example a 72 mm long screw with a diameter of 18 mm is a 4D screw. A variety of length to diameter L/D ratios can be purchased, typically in the range 24 to 45. Modular machines are usually built in blocks of typically 4 or 5 D.

High-speed co-rotating extruders have a closely matching flight profile. There is a considerable open area from one channel to the adjacent channel. The assembly can therefore be designed with a relatively small clearance between the two screws; the screws are then closely self-wiping. Twin-screws of this design are generally referred to as closely self-wiping co-rotating extruders.

Since the tendency to develop large pressure peaks in the intermeshing region is quite small, the closely self-wiping co-rotating extruders can run at high speeds, usually higher than 600 rpm. Fluid regions at different locations will have different velocities when flowing inside the screw channel. Therefore the time spent, by a discrete element of fluid passing through the channel will be different depending on starting position. The time taken for material to travel along the screw is known as the residence time. So there is a distribution of residence times dependent upon the starting point. However, this geometrical characteristic also results in reduced conveyaning with a corresponding wide distribution of residence times and [pressure-sensitive throughput]?.

The conveying and mixing characteristics of intermeshing co-rotating twin-screw extruders are attributed to the geometry of the elements. An open screw channel exists in the axial direction (parallel to the screw axis), and provides the possibility of axial mixing in a lengthwise direction. The screw channel can be either crosswise closed with screw elements or crosswise open with kneading discs. Various combinations of screw elements and kneading discs can be arranged according to mixing requirements. One special characteristic of intermeshing co-rotating systems with self-wiping profiles is the narrow distribution of residence time because it is difficult for materials to stay at the barrel surface or screw flanks and roots.

1.3.1 Screw Elements

Screw Elements are the most important element for the configuration of the process taking place in the TSE. By modifying the order of screw elements along the direction of material flow through the extruder, the mixing and conveying characteristics can be altered over very broad range.

The following table gives an overview of the general characteristics of the three main types of elements. Table 1-3-1

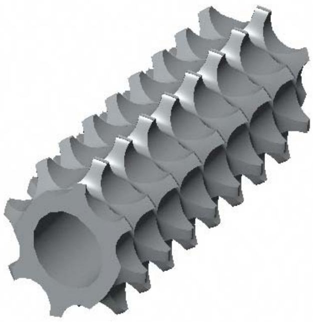
Type of element	Main function	Main characteristics
	Conveying Pressure built-up	• Limited mixing • Short residence time
	Dispersive Mixing	• Low/Zero pressure built-up • Medium to long residence time
	Distributive Mixing	• Low/Zero pressure built-up • Medium to long residence time

Table 1-3-1: Standard screw elements for TSE

In the configuration of a typical compounding screw these elements are almost always used in a special configuration using tailored sequences of elements, where the sequence mainly depends on the general processing concept.

Typically the main functions of a compounding screw for a filled or reinforced system are:

1. Melting the base polymer and the necessary additives
2. Side feeding of the filler or the fibres
3. Atmospheric venting for the stripping of air that was taken in by the filler/fibres
4. Incorporation of the fibres/Dispersion of the filler
5. Vacuum degassing
6. Pressure build-up for the pumping of the compound through the die.

The following figure 1-3-1 shows a typical screw set-up for compounding of a filler-containing compound, incorporating the processing steps mentioned above.

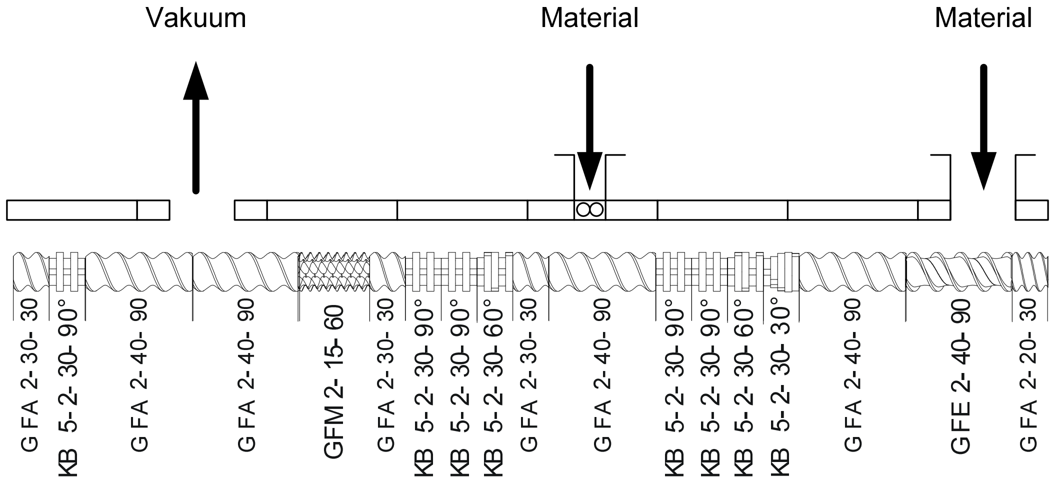


Figure 1-3-1: Typically compounding screw setup.

Depending on the nature of the polymer, the filler, the viscosity, the size of the machine, the installed maximum torque and the individual philosophy of the compounder the screw needs to be modified individually. Often there is more than one suitable compounding screw configuration and in the end it is up to the individual philosophy and also the need for the flexibility or universality of the screw that finally determines the screw profile.

1.3.2 Barrel elements

For the configuration of the barrel there are typical standard closed barrel blocks available as well as some variations to fulfil the material feeding and melt degassing functions illustrated in figure 1-3-2.

Typically closed blocks (figure 1-3-2) are used in the melting and mixing areas. In machines that are used flexibly for different material systems the degassing blocks can be closed with plugs if no degassing is required.

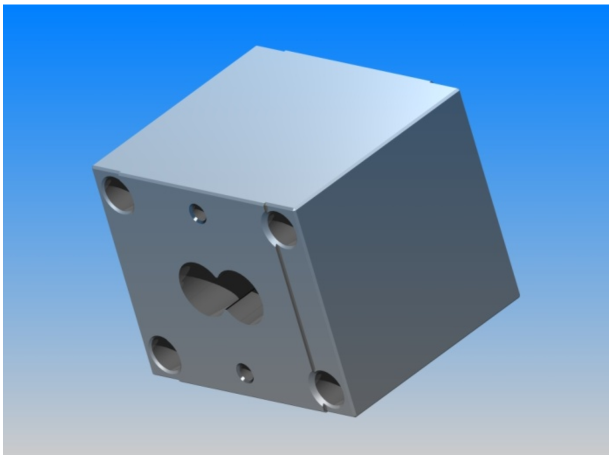


Figure 1-3-2: Typical closed barrel block

Degassing blocks (figure 1-3-3) are used to strip low molecular weight components out of the melt. Typically, there are inserts available with special degassing geometries that fit into the illustrated large opening. These inserts help to keep the melt in the barrel and allow a way out for the gas.

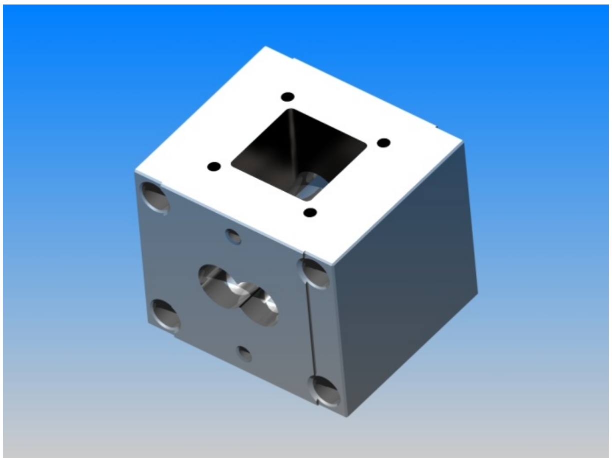


Figure 1-3-3: Typical degassing block

If a separate material stream should be fed into the molten polymer, then side feeders are used. For the addition of side feeder's special blocks are available, as illustrated in figure 1-3-4. These blocks often offer a venting port on the top that allows air that has been taken in by the side feeder to escape.

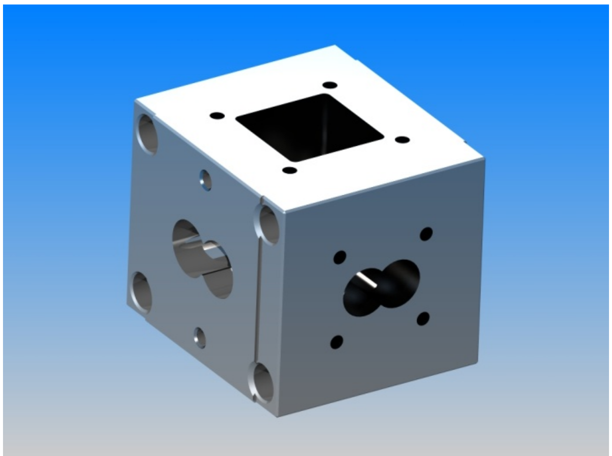
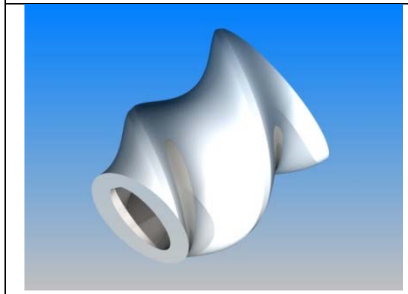
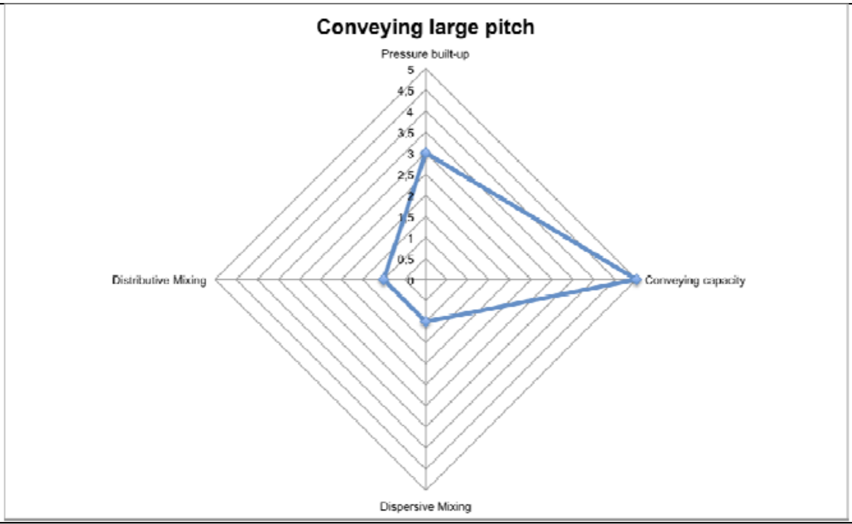
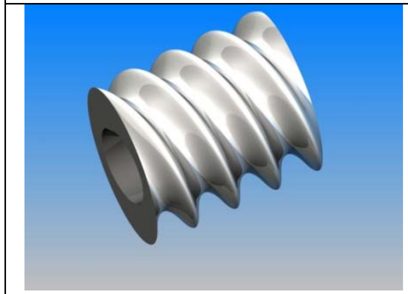
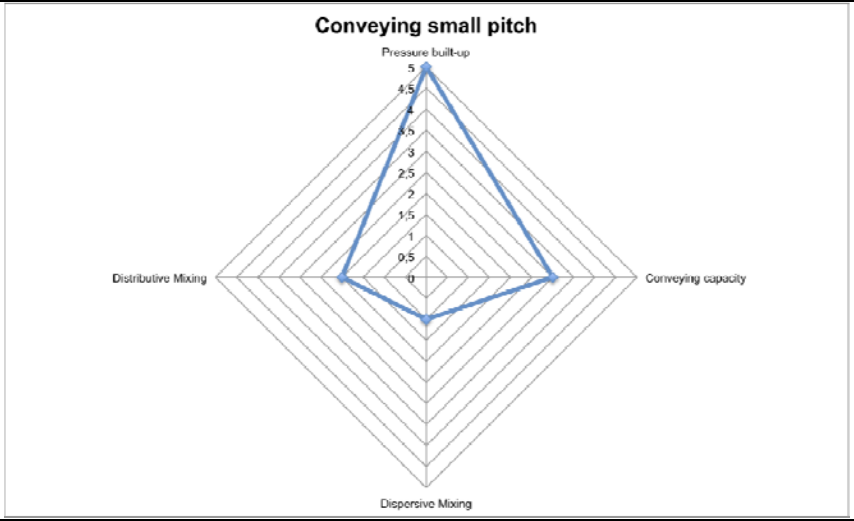


Figure 1-3-4: Typical side feeding block

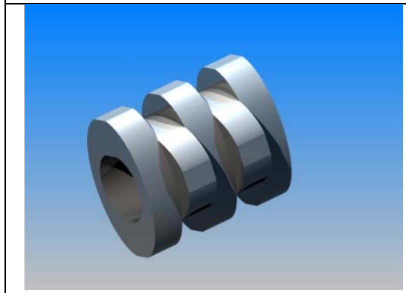
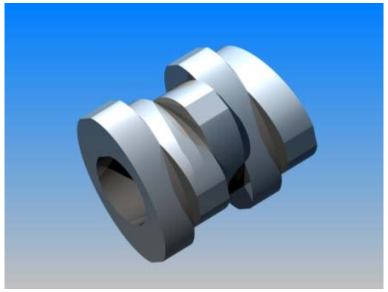
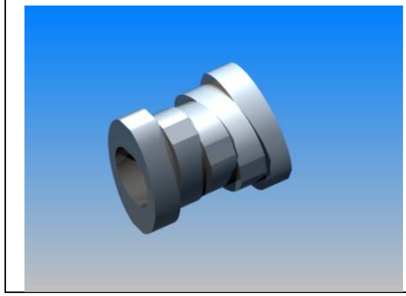
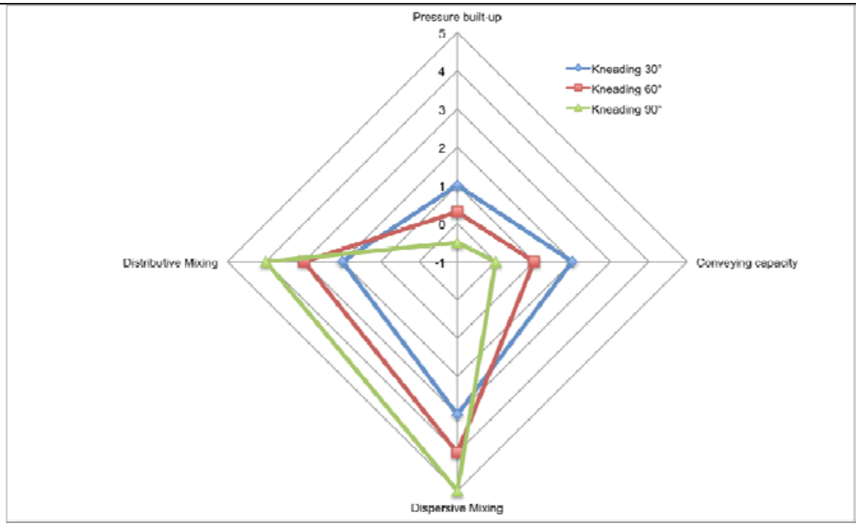
1.4 Ways to approach the optimum compounding screw configuration

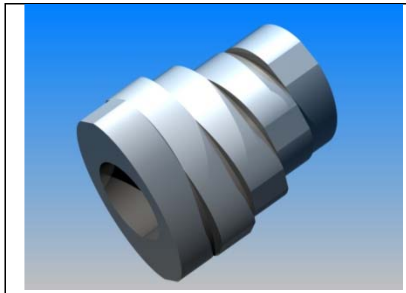
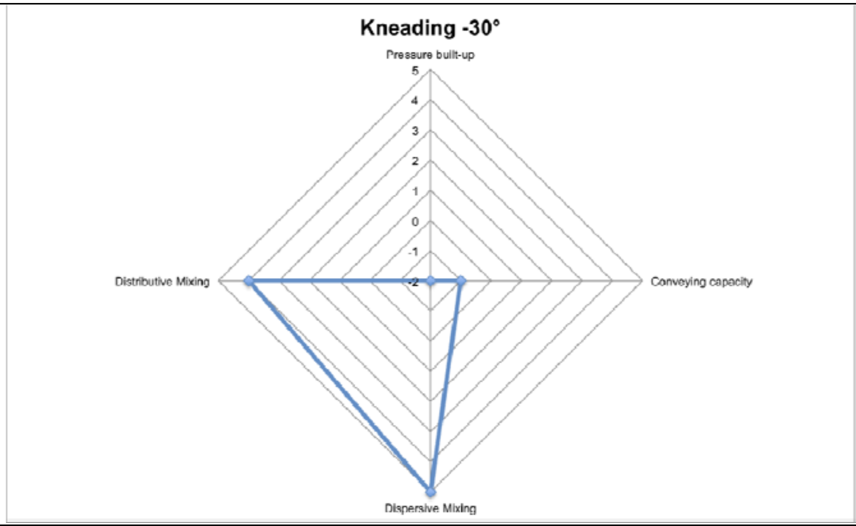
There a several ways to approach a more or less optimum screw configuration. Today's state of the art in the typical compounding business is the use of the extensive experience of both the processor and the machine manufacturer to determine a good initial screw configuration that normally allows production of the desired type for compound. For this initial configuration the qualitative characterisation of the most common screw elements shown in table 1-4-1 can be used:

1.4.1 Table 1-4-1: Processing Characteristics of Conveying Element

Element	Characteristics	Remarks
		Mixing characteristic strongly depends on: The pressure the element has to build up The fill ratio of the element
		Mixing characteristic strongly depends on the pressure the element has to build up and the fill ratio. Conveying capacity can be to small to pump the material coming from larger pitch upstream elements. In this case the small pitched conveying element will become a pressure consumer.

1.4.2 Table 1-4-1: Processing Characteristics of Kneading discs

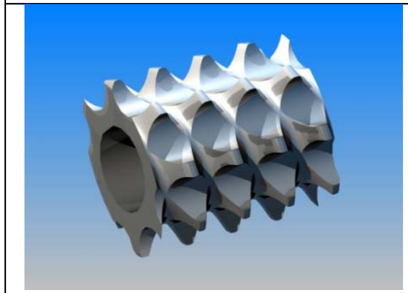
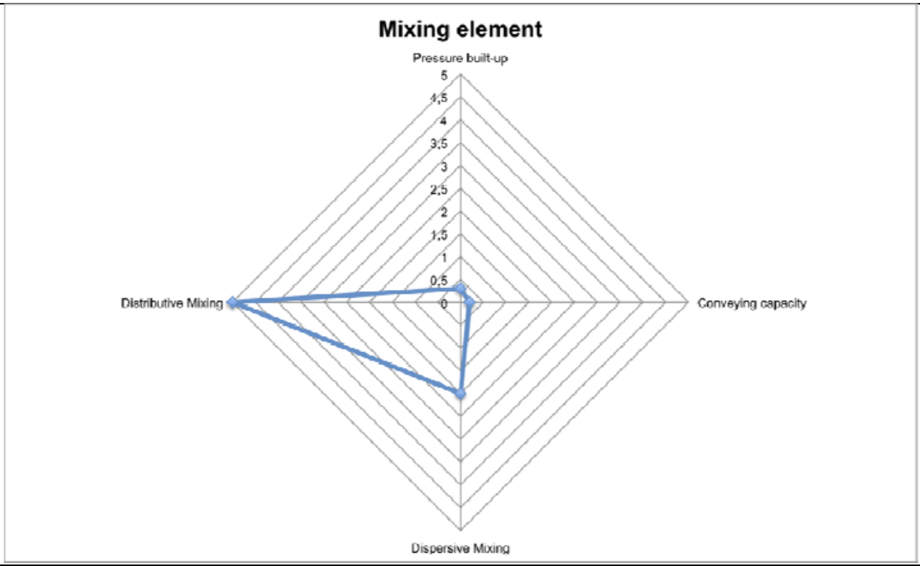
Element	Characteristics	Remarks
  		Mixing efficiency is not influenced by the static pressure in the element. Mixing efficiency does depend on the throughput, because as a fully filled element, the throughput influences the residence time and therefore the total mixing energy input.

<table>
<tr>
<td></td>
<td>
</td>
<td>Mixing efficiency is not influenced by the static pressure in the element.

Mixing efficiency depends on the throughput, because as a fully filled element the throughput influences the residence time and therefore the total mixing energy input.

Overall mixing characteristic is very similar to the 90° kneading block</td>
</tr>
</table>

1.4.3 Table 1-4-1: Processing Characteristics of Mixing elements

Element	Characteristics	Remarks
		Mixing and conveying efficiency is mostly affected by the final geometry of the element.

Based on this initial screw concept, trials are normally carried out to optimise both:

- Material quality. Here, several very different properties might be focused upon, for example: Mechanical properties, Dispersion factors, Material degradation, colour or other properties that might be influenced by the state of dispersion and the material degradation
- Output. In almost every case the desired technical properties should be achieved at maximum output. Therefore often a quality versus output test is also carried out to determine how screw speed and feed-rate in combination with the individual process configuration is interacting.

This process of optimisation can be a quite time and material consuming process

1.5 Typical conventional measures to improve the processing setup

Besides the described characterisation of the achieved compounded material, further characterisation methods are available to achieve better process understanding for a more targeted process optimisation.

Some of the most important measures are described in the following chapters.

1.5.1 Local Temperature measurement

In cases where the temperature stability of the material system is very limited or extensive shear might cause local temperature peaks it is possible to build up the barrel with several venting ports that are normally closed. During normal operation these venting ports can be briefly opened and with an infrared temperature gauge the local melt temperature can be determined in the different sections of the screw. These venting ports need to be located carefully in the barrel design otherwise to much melt may escape from the barrel in these sections. Therefore it is best to place them directly after a kneading disc section.

With these additional 3-5 temperatures, the optimisation of the kneading disc sections can be speeded up. The temperature increase can be determined and material samples can be taken to characterise the dispersion level along the material flow path.

1.5.2 Local sampling barrels

For some lab-scale machines specially designed barrels are available that allow local material samples to taken in every barrel segment (usually 4D long). These local material samples can be analysed for their dispersion state and degradation to help optimise the screw set-up

1.5.3 Lab-Scale machines with divided barrels or extractable screws

These machines are available from some lab-equipment extruder manufacturers. In principal there are two concepts on the market.

One adapts a divided barrel that can be opened horizontally. Such a machine concept is illustrated in figure 1-5-1

Figure 1-5-1: Extruder with horizontally divided barrel. Source: www.brabender.com

The second concept has an automation device for the extraction of the screws to the rear on an extended machine bed (see figure 1-5-2)

Figure 1-5-2: Extruder with extractable screw. Source: www.berstorff.de

Both machines allow the operator to stop the process and to take local material samples to analyse material quality, degradation and mixing efficiency in the individual screw sections.

In both cases this does not work with material systems that rapidly re-agglomeration or phase separate, because this is the time that is needed to extract the screws.

On the other hand these systems allow a more detailed look on the processing characteristics of the individual zone, because for example the fill level of the element can be judged quite precisely.

1.5.4 Using transparent barrels

Transparent barrels have been used for quite some time to understand the flow characteristics in certain screw geometries.

Examples are shown in figure 1-5-3 and 1-5-4.

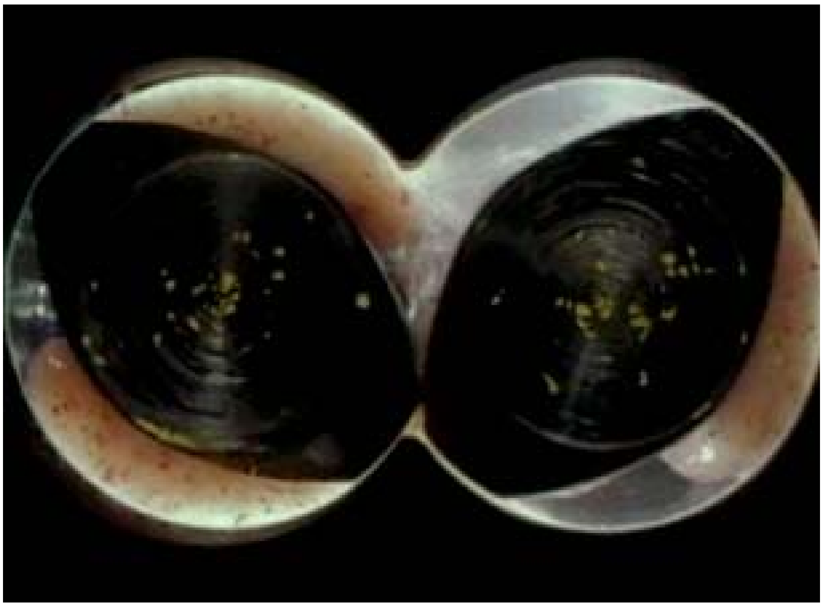


Figure 1-5-3: Glass barrel with screw cross-section.
Source Coperion, Stuttgart

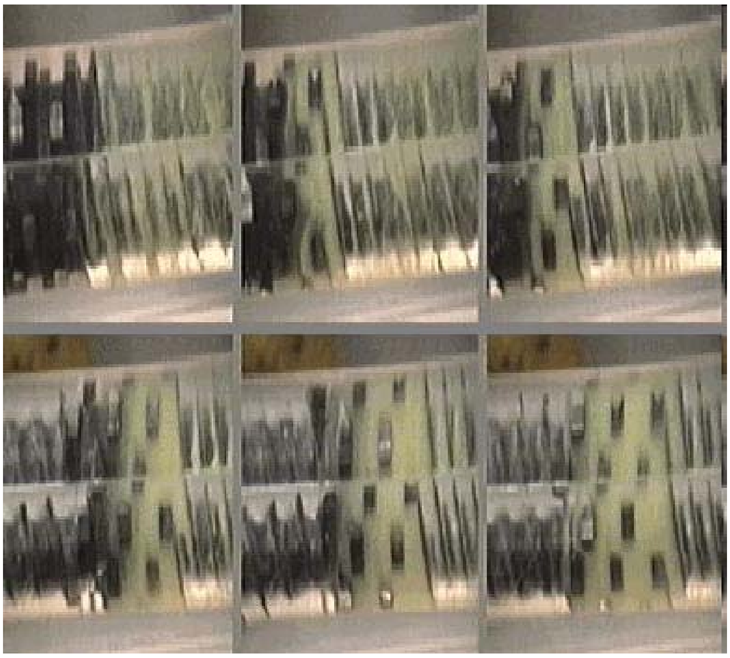


Figure 1-5-4: Glass barrel with kneading disc section.
Source: www.dep.uminho.pt

These transparent barrels help to understand the general flow pattern within standard geometries, but they are not suitable to improve the processing of individual material systems. This is mainly due to the transparent barrel materials not being capable of withstanding the processing temperatures or pressures of conventional thermoplastics.

2 Potential and Limitations of PEPTflow

2.1 PEPTFlow Visualisation Technology

PEPTFlow is concerned with the application of PEPT (Positron Emission Particle Tracking) to polymer flow in twin-screw extrusion. PEPT is a unique non-intrusive experimental technique that uses radioactive tracer particles to measure flow within real processing equipment. The method has been exploited predominantly in granular systems but also in liquid systems. In viscous, low Reynolds Number polymer flow, the trajectories are taken to be representative of streamlines and can be used to infer mixing and dispersion.

The experimental set-up was based on a Leistritz Micro 27 mm twin-screw extruder that was modified by partners ICT Fraunhofer and Extricom to provide a PEPT window as reported in Deliverable D7. Studies showed that the thick steel of the extruder barrel was effectively impenetrable to gamma photons. For PEPT to work therefore, a section of barrel with reduced wall mass was required. This was provided by a surface hardened aluminium insert with nominal wall thickness of 25mm. The length of the exposed aluminium section, 110mm, gave a field of view of approximately 90mm. The design of the PEPT window was a considered compromise between exposed length (i.e. field of view) and PEPT reliability. The latter requires low wall thickness to minimize photon scatter while a longer field of view requires a larger wall thickness to resist the twisting forces imparted by the screws. Other materials of construction were considered, and tested (such as ceramic) but were not deemed suitable.

The modular PEPT camera, specifically designed for the modified extruder was manufactured, installed and commissioned. The completed set-up is shown in Figure 2-1-1.

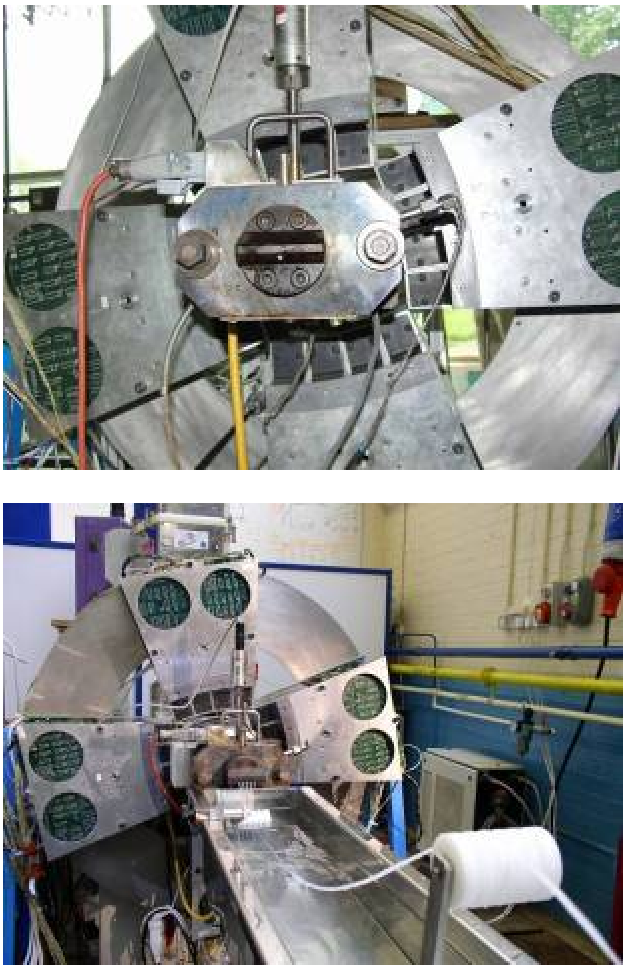


Figure 2-1-1 - The PEPTFlow extruder with modular PEPT camera

A comprehensive experimental plan was designed to maximise the range of conditions investigated within the measurement time available. This is discussed in Section 2.

Positron Emission Particle Tracking generates trajectory data initially as a list of co-ordinates of the paired gamma photons detected as the tracer moves through the field of view. Electronic circuitry within the camera, termed “coincidence boards”, pair the photons according to detection time. Each detected pair is known as an “event” and the line connecting them is termed a line of response (LOR). Events are generated at rates up to 10^6 Hz (1 MHz) and particle locations are obtained from triangulation of the lines of response collected over a period of a few milliseconds. The data however comprises a mixture of true and so-called “corrupted” events. The latter arise from photon scattering or invalid pairing, and will reduce the certainty of location measurement. It is not possible to determine *a priori* which pairs are true and which are corrupted (although a proportion of photons are sufficiently scattered that they can be eliminated because the consequent energy loss is detectable and measured by the camera). A statistical algorithm is therefore used to home in on the most convergent point of the lines by iteratively removing outliers. This requires the selection of parameters such as how many events to use for each location and how many to discard during iteration. This is covered in more detail in Section 4.

The algorithm delivers the trajectory in the form of an ASCII file showing the three dimensional location of the particle at discrete time steps. For a given equipment geometry, the frequency at which locations are generated is mainly dependent on the tracer activity which is dependent on the age, the number of times the tracer has been used, as well as the initial activity achieved. The consequence of this is that there is a spread in the “quality” of the data. Some of the runs give very high data frequency (few milliseconds between data points) while others give longer time steps, up to 20 milliseconds or longer.

The PEPTFlow field of view is illustrated in figure 2-1-1, showing the barrel in-liner and the location of the elements underneath this window:

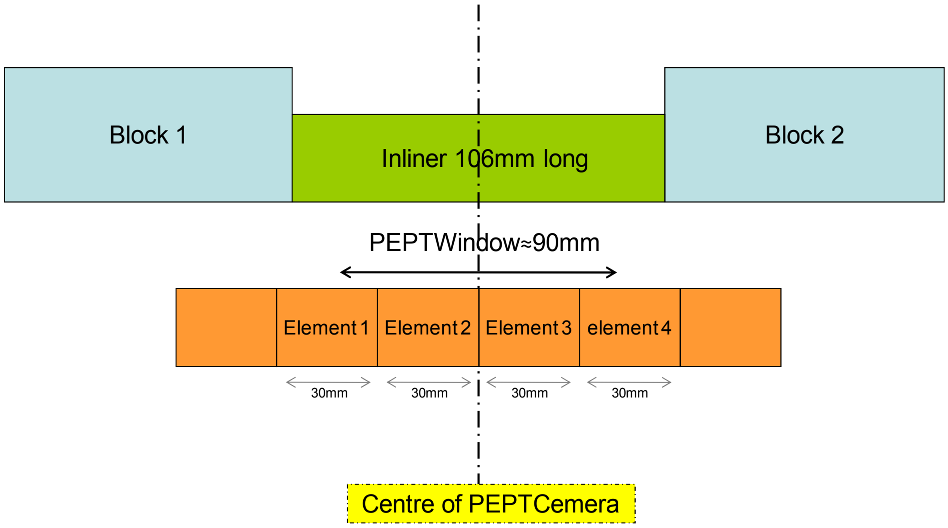


Figure 2-1-2: Field of view and location of the screw elements

In practice only the data collected in Element 2 and 3 is complete data for a whole screw element. Data for element 1 and 4 sometimes only covers a few millimetres of screw element length.

2.2 Data Analysis

The basic principal of PEPT, as previously described, is to locate the position of a radioactive particle by triangulation of gamma photon radiation, as illustrated in figure 2-2-1

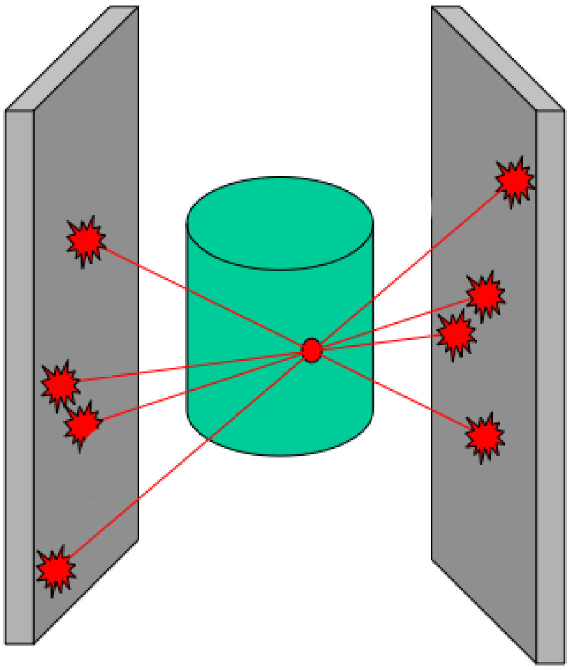


Figure 2-2-1: Particle position tracking principal

After careful data-processing, that mainly eliminates outliers and noise, this tracer location over time can then be plotted in 3D graphs, showing the individual trajectory of this passage. Although this graph is not really suitable for quantitative comparisons, it can be very useful to determine special flow conditions (see figure 2-2-2). In this individual run the particle became ‘stuck’ for quite some time on one of the compounding screws.

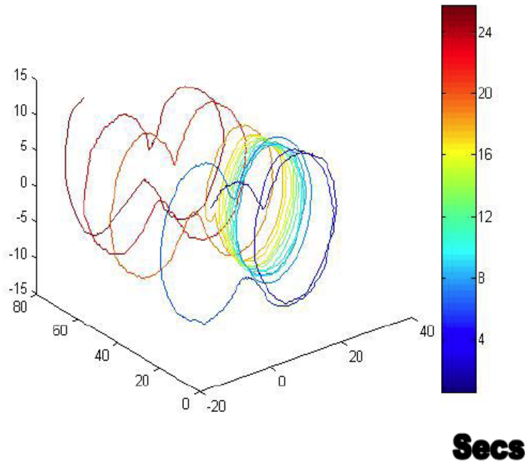


Figure 2-2-2: 3D graph of the tracer position

Plotting the X-, Y-, Z-coordinates versus time as illustrated in figure 2-2-3 gives another perspective on the same data.

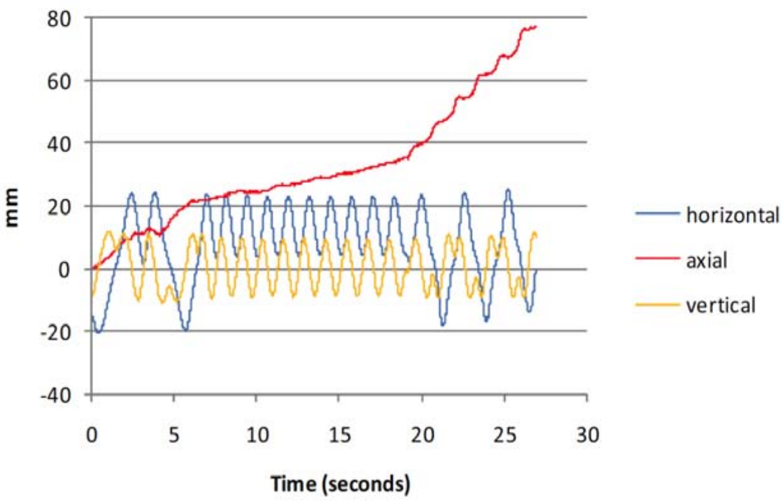


Figure 2-2-3: XYZ coordinates versus time

Plotting the XY-coordinates versus the Z-distance give a realistic picture of the projection of the tracer movement, that especially demonstrates areas of fast and slow movement (see figure 2-2-4).

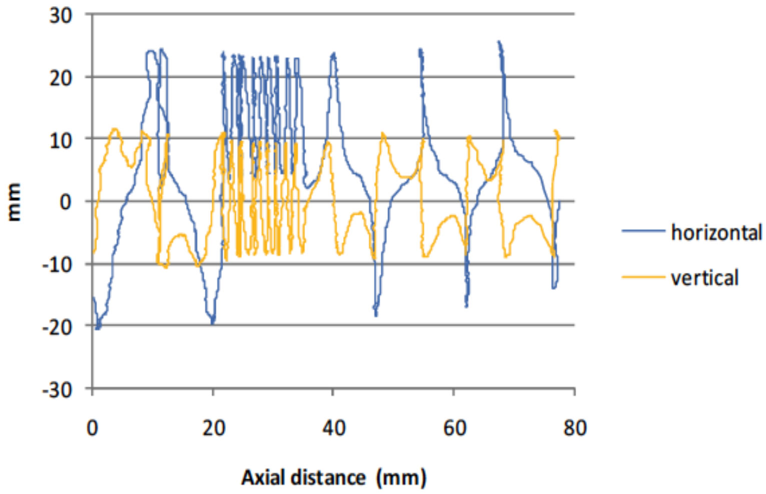


Figure 2-2-4: XY-coordinates over Z

Plotting the XY-Coordinates in an XY Diagram gives the axial projection of the flow path, which can deliver valuable information about where the particle was located for a certain time, if it passed between the screws or became stuck to the barrel or the screw (see figure 2-2-5).

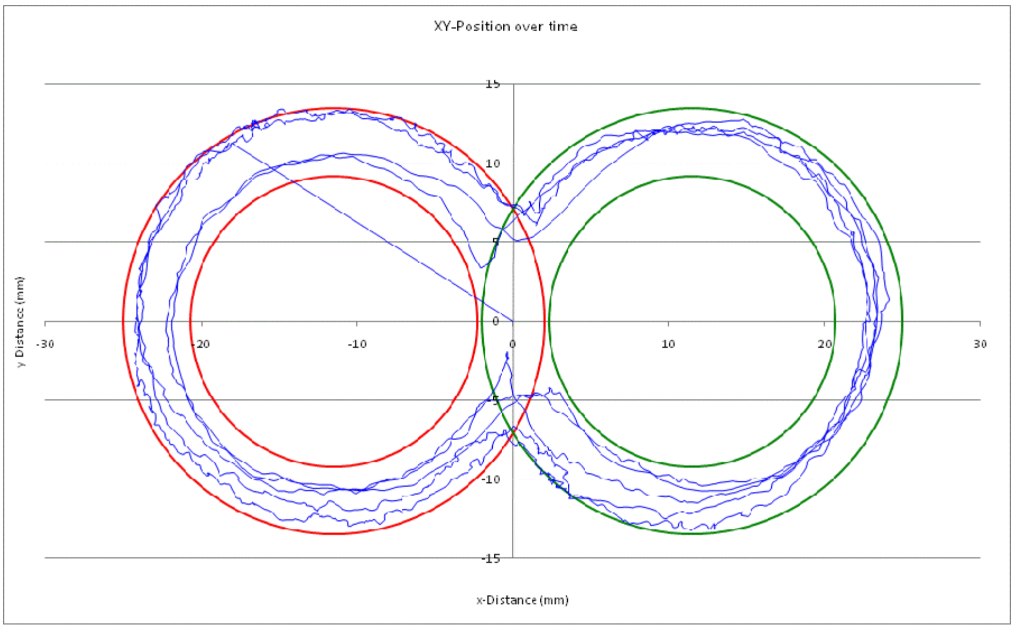


Figure 2-2-5: XY-Coordinates versus time

Based on a extensive EXCEL-Spreadsheet calculation the speed of the particle can be illustrated in a velocity over z graph (see figure 2-2-6)

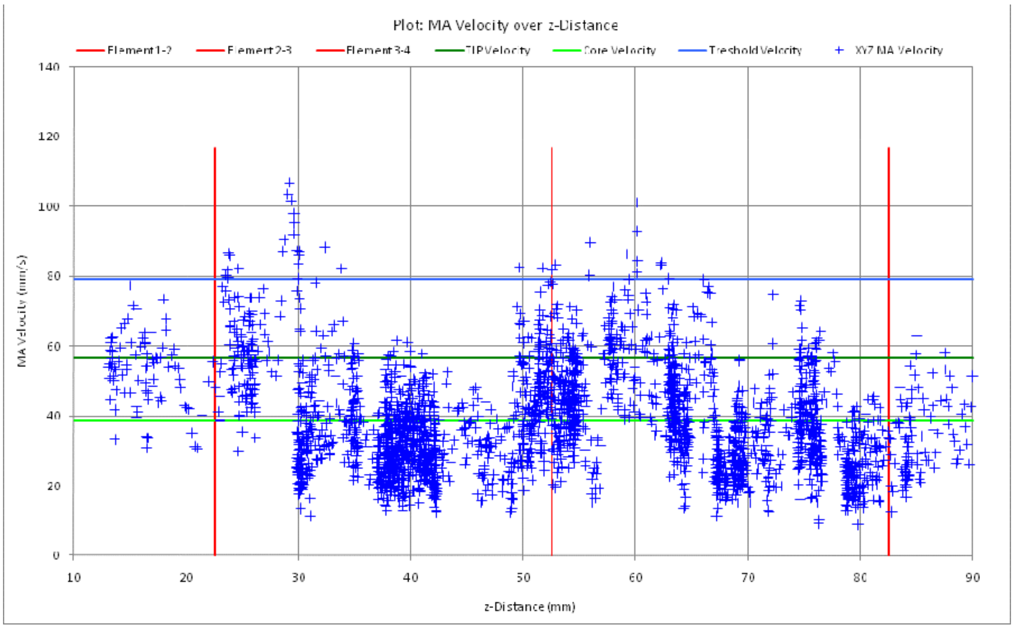


Figure 2-2-6: Moving Average smoothed velocity versus z-Distance

This graph shows the differences in particle speed that can be linked in some way to the mixing capabilities of the screw section. Furthermore, it also often shows clear signs of the movement of the particle. For example the chosen graph clearly shows that the particle is moving stepwise in the z direction whereas the velocity is changing constantly.

Furthermore, this table calculates average values for the characteristics of the individual run (see following table 2-2-1 for some details).

Value	Unit	Description
time		
Min	s	Should always be zero
Max	s	Time for the total passage, calculated based on the sum of delta t
z-value		
Min	mm	First position reading in section
Max	mm	Last position reading in section
error		
Min		
Max		
Delta t		
Average	s	Average time period between position readings
Median	s	Median value of time period (alternative average)
Average Deviation	s	
Standard Deviation	s	
Min	s	Min delta t
Max	s	Max delta t
Sum	s	See above
Delta XY		
Average	mm	Average XY step length between postions
Median	mm	
Average Deviation	mm	
Standard Deviation	mm	
Min	mm	Min step length in XY direction
Max	mm	Max step length in XY direction
Sum	mm	Total trajectory length in XY projection section
Delta XYZ		
Average	mm	Average XYZ step length between postions
Median	mm	
Average Deviation	mm	
Standard Deviation	mm	Standard deviation of XYZ step length (could be something like melt velocity variation?)
Min	mm	Min step length in XYZ direction
Max	mm	Max step length in XYZ direction
Sum	mm	Total trajectory length in XYZ projection section
XYZ Velocity		Velocities calculated based on unsmoothed data
Average	mm/s	
Median	mm/s	
Average Deviation	mm/s	
Standard Deviation	mm/s	
Min	mm/s	
Max	mm/s	
Sum	mm/s	
XYZ MA Velocity		Velocities calculated based on smoothed data (Moving average of 2 velocities)
Average	mm/s	
Median	mm/s	
Average Deviation	mm/s	
Standard Deviation	mm/s	
Min	mm/s	
Max	mm/s	
Sum	mm/s	
XYZ Accel		Acceleration calculated based on unsmoothed data
Average	mm/s2	
Median	mm/s2	
Average Deviation	mm/s2	
Standard Deviation	mm/s2	
Min	mm/s2	
Max	mm/s2	
Sum	mm/s2	

XYZ MA Accel		Acceleration calculated based on smoothed data (Moving average of 2 velocities)
Average	mm/s2	
Median	mm/s2	
Average Deviation	mm/s2	
Standard Deviation	mm/s2	
Min	mm/s2	
Max	mm/s2	
Sum	mm/s2	
Ratios		
XY / XYZ		Ratio of XY flow path length versus XYZ flow path length
XYZ / t		XYZ flow path length versus passage time for the section
Quaters		
Sum Q1/Total Section		Relative Number of position readings in Q1
Sum Q2/Total Section		Relative Number of position readings in Q2
Sum Q3/Total Section		Relative Number of position readings in Q3
Sum Q4/Total Section		Relative Number of position readings in Q4
Sum Q1+Q2 (LHS from die)		Relative Number of position reading in Q1+Q2
Sum Q3+Q4 (RHS from die)		Relative Number of position reading in Q3+Q4
Total Sum		Total Number of Positions
Ratio (Q12 LHS / Q34 RHS)		Ration of (Q1_2/Q3_4)
Time Q1/time section		Relative Time spent in Q1
Time Q2/time section		Relative Time spent in Q2
Time Q3/time section		Relative Time spent in Q3
Time Q4/time section		Relative Time spent in Q4
Sum Q1+Q2 (LHS)		Relative time in Q1+Q2
Sum Q3+Q4 (RHS)		Relative time in Q3+Q4
Ratio (Q12 LHS / Q34 RHS)		Ration of (Q1_2/Q3_4)
Passages		
Number of PbS		Passages between screws
Number from StS		Total number of jumps from screw to screw
Number PbS/Cycles		Ratio of Passages between screws vs total cycles
XYZ Velocity > v Tip		Number of positions were UNSMOOTHED XYZ velocity exceeds tip-velocity
v MA > vTip		Number of positions were SMOOTHED XYZ velocity exceeds tip-velocity
XYZ Velocity > vTresh		Number of positions were UNSMOOTHED XYZ velocity exceeds defined velocity
v MA > vTresh		Number of positions were SMOOTHED XYZ velocity exceeds defined velocity
r > rTRESH		Number of positions which have a RADIUS larger then defined radius
TipPass		Total number of positions where vXYZ>vTip AND r>rTresh
Ratio XYZ velocity > vTip		Numbers of vMA>vTip divided by total number of Positions
Ratio MA > vTip		Numbers of XYZ Velocity>vTip divided by total number of Positions
Ratio XYZ velocity > vTresh		Numbers of XYZ Velocity>vTresh divided by total number of Positions
Ratio v MA > vTresh		Numbers of vMA>vTresh divided by total number of Positions
Ratio > rTresh		Numbers of r>rTresh divided by total number of Positions
Ration TipPass		Numbers of TipPass divided by total number of Positions

Table 2-2-1: Values calculated by the run-spreatsheet

2.3 Analysis of several trajectories of one experiment

Having analysed each run within a particular experiment, then another spreadsheet template was used to summarise all of the runs for that experiment. This summary contained the items listed in Table 2-3-1. One important item however, was the coefficient of variation, which is explained in the following extract.

This summary template was used for each experiment to collect the key data from each run within that experiment, and to prepare an overview of the experiment in question. In this way, by using the residence time for each run, a statistical analysis can be carried out on the residence times giving a mean, median, and standard deviation for each experiment. This can also be separated out to cover each of the two elements under the Pept window.

Variable	Comment
Number of runs (N)	This will affect the degree of confidence of the results
Standard error	(1/√N) A measure of error due to the number of samples
Rt Mean (secs)	The numeric average
Rt Median (secs)	Midpoint of the data. If close to Mean = an even distribution
Rt Standard deviation	A measure of the spread and indication of distributive mixing
Rt Coefficient of Variation (SD/Mean)	This enables us to compare elements with different Means A dimensionless number for end to end distributive mixing
XY/XYZ	An indication of side to side mixing
XY/XYZ Std Deviation	A measure of the spread
XY/XYZ Coef. Of Variation	A dimensionless number to enable comparisons
Average velocity (mm/s)	As the clearances are the same for all elements this gives an indication of higher or lower shear rates.
Max acceleration (mm^2/s)k	This may indicate high or low stretching flows and hence Dispersive mixing.
Occupancy left/right	A measure of the work done on each screw
Passes between screws (Pbs)	An interesting number to look at as many people expect nothing to go between the screws, some expect lots!
Tip passes	This is an important number for dispersion
Pbs + Tip passes	Both may be important for dispersion, so add them together
Ratio velocity>threshold	Do we have many particles going faster than we expect?
% Tip passes	This is a dimensionless version to enable comparisons

Table 2-3-1 Summary data collected for each experiment.

2.4 Comparing Experiments

The spreadsheet delivers the residence time distribution for the whole PEPT-Window in the extruder (about 2,5 D long, see figure 2-4-1)

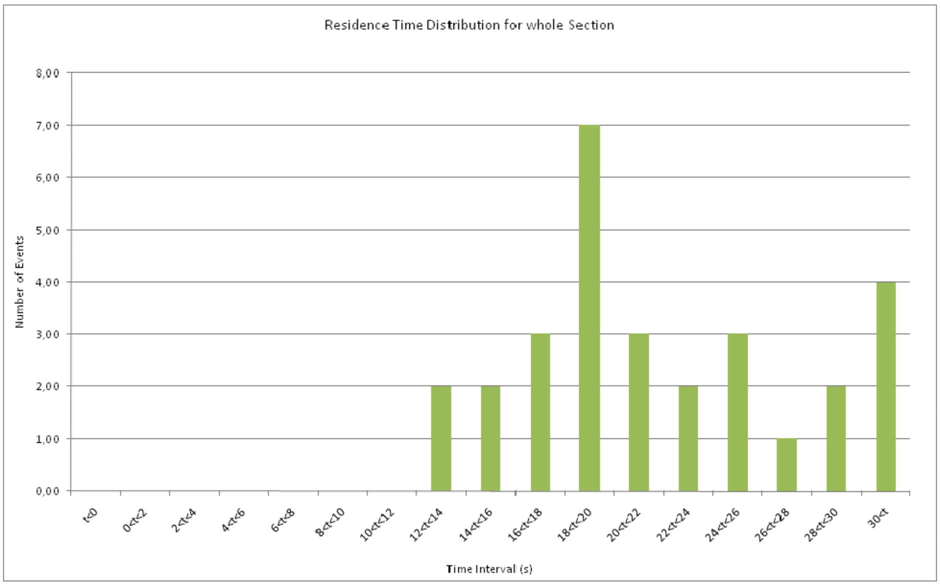


Figure 2-4-1: Residence time distribution for the whole data of the run (containing some data from element 1 and 4)

And locally separated into each individual element (see figure 2-4-2)

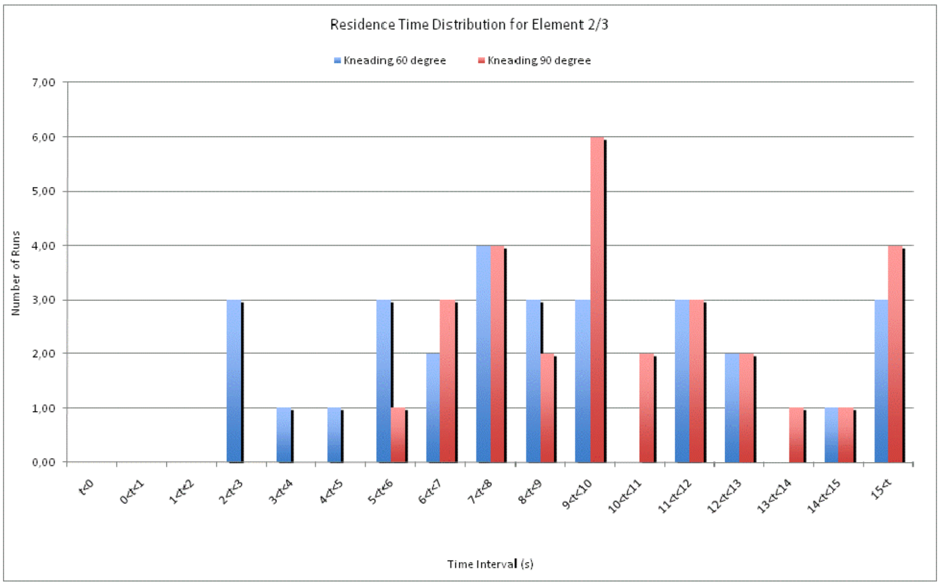


Figure 2-4-2: Residence time distribution for element 2 and 3

Especially the later diagram allows very interesting interpretations and delivers very valuable information for process optimisation, because the effect of different processing conditions, different materials and different pressure levels on the residence time distribution can clearly be seen in these diagrams. This is important information for everybody processing temperature and shear sensitive materials.

An additional spreadsheet was used to compare 2 experiments to each other.

In particular this spreadsheet compares those average values of the two conditions that are most representative for the individual experiment. The most important graphs are shown below.

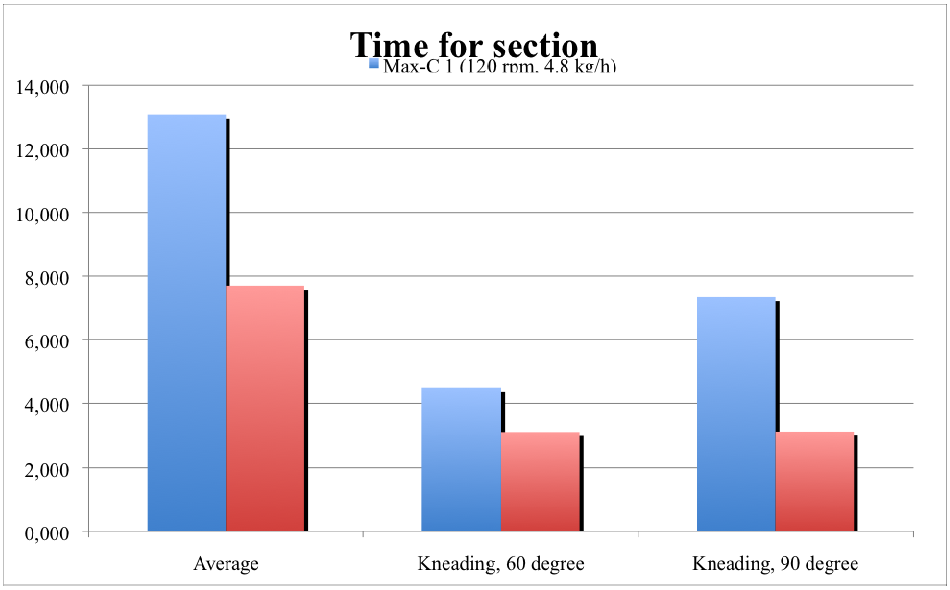


Figure 2-4-3: Total time for the passage of the individual section

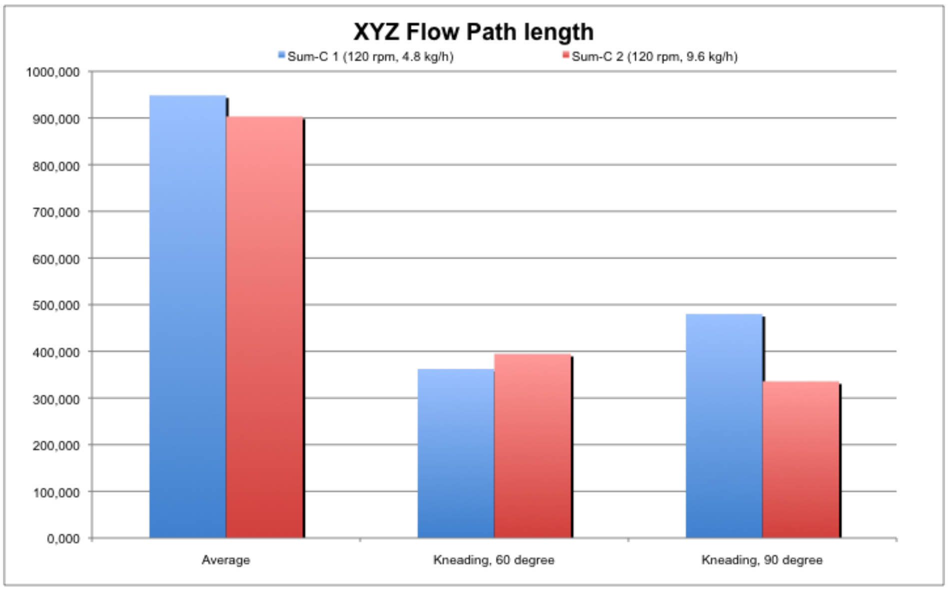


Figure 2-4-4: Flow path/trajectory length

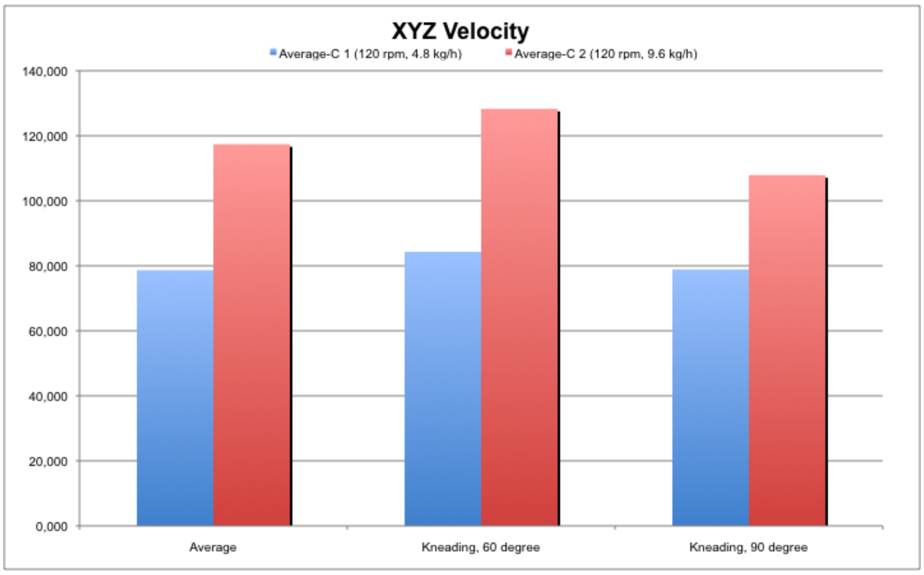


Figure 2-4-5: 3D Velocity in the individual element

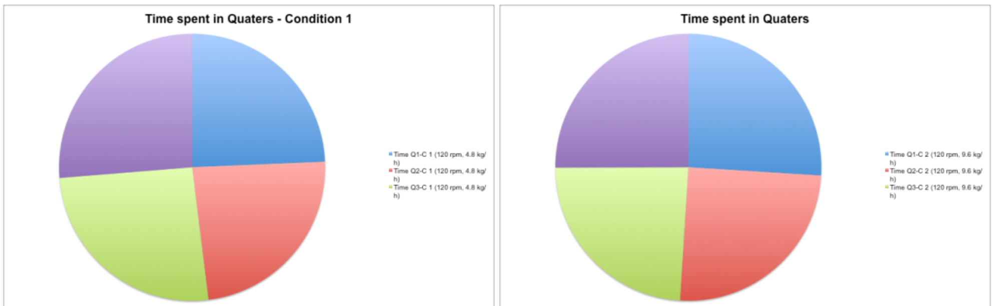


Figure 2-4-6: Time the particle spent in the individual quarter for experiment A and experiment B

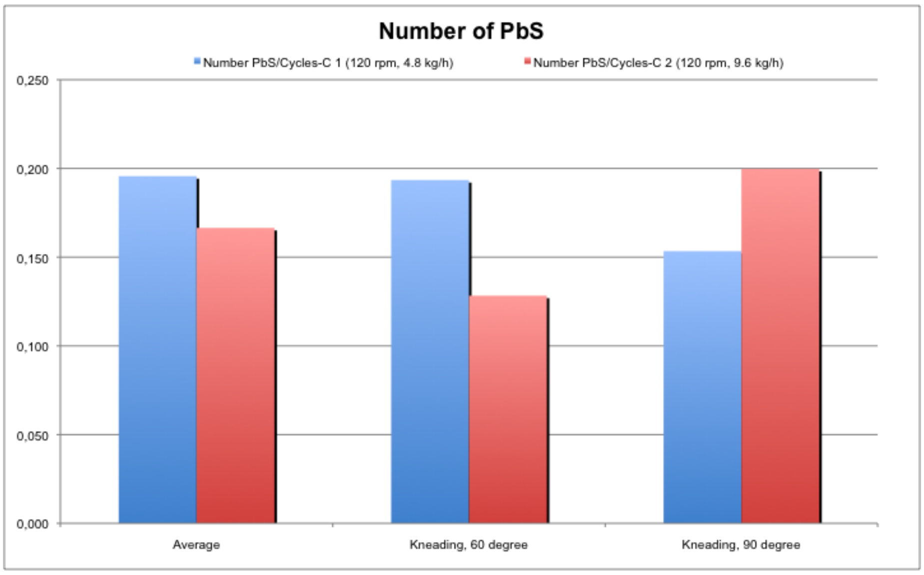


Figure 2-4-7: Relative Number of the Passages between the screws for the two experiments

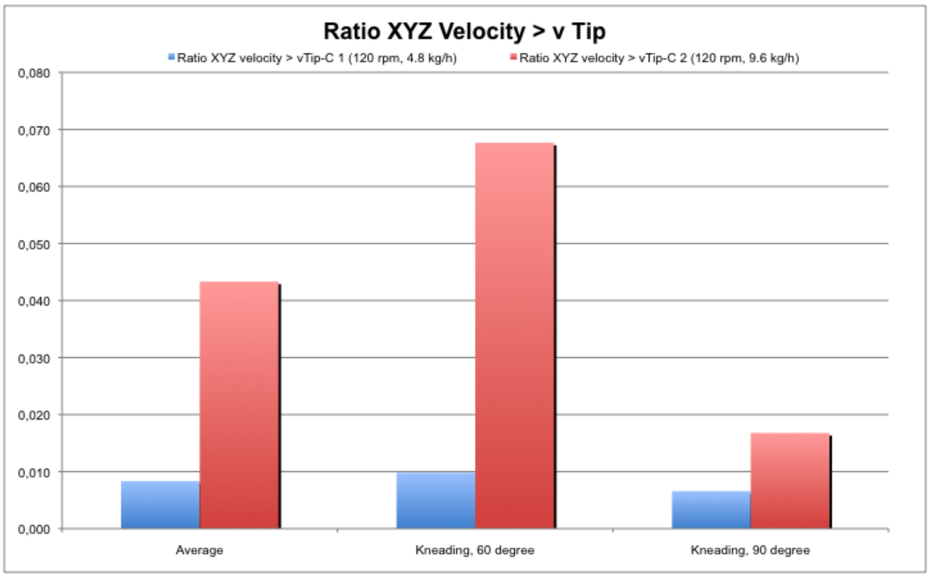


Figure 2-4-8: Relative Number of events, where the 3D Velocity is larger than the tip-velocity

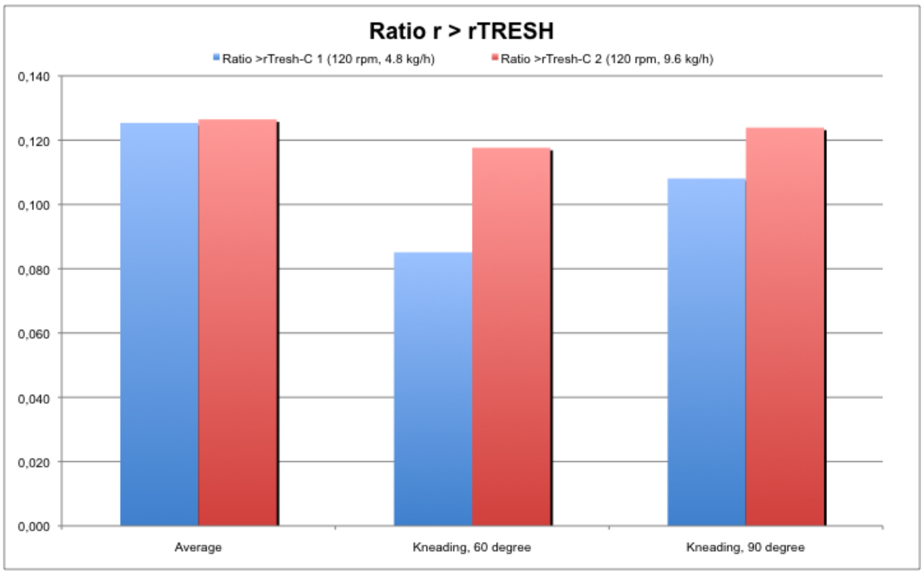


Figure 2-4-9: Relative Number of events where the particle is very near to the barrel surface.

These graphs in combination with the individual residence time distributions give a quite comprehensive and also measureable picture of the process taking place in the individual element under the defined processing conditions.

2.5 Summary of the possiblities of the current PEPTFlow technology

PEPTFlow is a completely new characterisation technology for polymer flow within polymer processing machines. It offers possiblities to gain insight into the machine that has never been possible before. On the other hand there are also some limitations, that one should know about when interpreting the results or thinking about using PEPTFlow technology for further flow analysis.

2.5.1 Potential

- PEPTFlow allows monitoring of polymer flow under realistic processing conditions
- PEPTFlow can monitor real polymers at high temperatures and high pressures.
- PEPTFlow allows monitoring of flow locally in individual screw elements

- PEPTFlow allows the calculation of residence time distributions, even for sections of screw elements
- PEPTFlow identifies regions with very long residence time

2.5.2 Limitations

- Due to the current limition on positional frequency and some necessary smoothing to avoid excessive noise, it is presently only reasonable to monitor screw speeds of up to 300 rpm.
- Only one particle can be traced in an individual run. Only 50-60 trajectories can be taken in one day.
- Currently, the field of view is limited to 2,5-3 D screw length (see picture of PEPT barrel 2-1-2)

3 Residence time in individual elements

3.1 The experimental plan

With three different conveying elements, three different sets of kneading blocks and a reversing element, the PEPTFlow project had a total of seven different elements to consider. It was felt that each one would be influenced by, not just the downstream element, but also the pumping capacity of the upstream element, and the adjacent configurations. The original ambition was to have four elements within the PEPT window, of which three would be fully covered, but it was found that we were only able to monitor the central pair of elements, with a small portion of the end of the first element and the start of the fourth element (See figure 3-1-1).

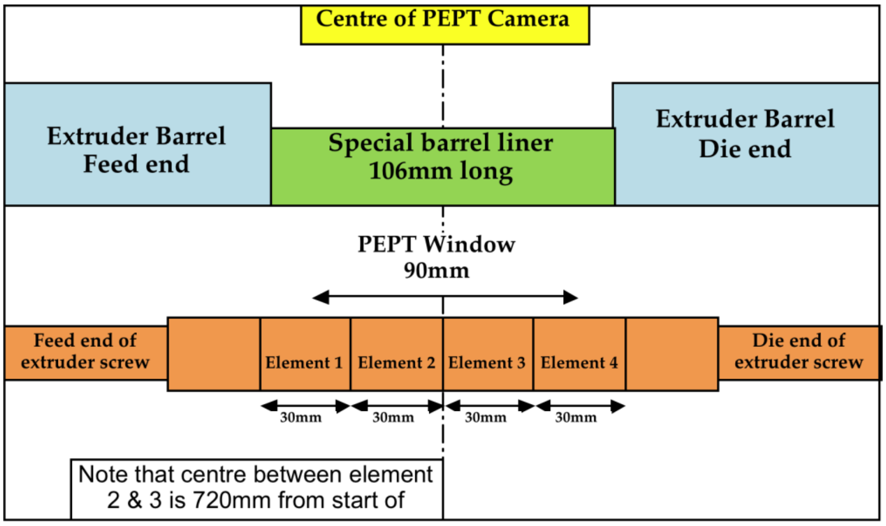


Figure 3-1-1: Dimensions and positions of the PEPTWindow

Hence, with the PEPT window covering only two elements, in order to examine all possibilities it would have been necessary to run an estimated 350 tests or more. There was clearly not enough time to complete this number of experiments, let alone analyse the data that would have been produced. We therefore agreed to run a range of configurations that we felt would` give us maximum information for minimum running time. The experiments carried out are summarised in table 3-1-1, and are discussed briefly below.

Each experiment typically comprises between 20 and 30 runs (passes of the tracer through the field of view). For several of the experiments this number was greatly exceeded. Experiments 14 and 15 for instance each comprised more than 100 runs. The data from each run has been processed and made available as individual Excel spreadsheets. This gave the time-stamped co-ordinates of the particle trajectory. A separate Excel file gave the angular position of the screw at each time step from the tachometer signal input.

Exp No.	Element 1	Element 2	Element 3	Elment 4	Polymer	Screw Speed (rpm)	Feed Rate (kg/hr)
1	C - 40mm	Mixing Element		C - 30mm	PP - MFI High	60	4.5
2	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	40	2.4
3	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	80	4.8
4	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	120	4.8
5	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	200	9.6
6	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	200	4.8
7	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	80	9.6
8	K 30°	K 60°	K 90°	C - 30mm	PP - MFI High	120	9.6
9	C - 40mm	C - 40mm	C - 30mm	C - 30mm	PP - MFI High	80	4.8
10	C - 40mm	C - 40mm	C - 30mm	C - 30mm	PP - MFI High	200	4.8
11	C - 40mm	C - 40mm	C - 30mm	C - 30mm	PP - MFI High	200	9.6
12	C - 40mm	C - 40mm	C - 30mm	C - 30mm	PP - MFI High	80	9.6
13	C - 40mm	C - 40mm	C - 30mm	C - 30mm	PP - MFI High	140	7.2
14	C - 30mm	C - 30mm	C - 30mm	RC - 20mm	PP - MFI High	80	4.8
15	C - 30mm	K 90°	K 90°	RC - 20mm	PP - MFI High	80	4.8
16	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI High	80	4.8
17	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI High	160	9.6
18	C - 30mm	C - 15mm	K 90°	K 90°	PP - MFI High	80	4.8
19	C - 30mm	C - 15mm	K 90°	K 90°	PP - MFI High	160	9.6
20	C - 30mm	C - 30mm	K 30°	K 30°	PP - MFI High	80	4.8
21	C - 30mm	C - 30mm	K 30°	K 30°	PP - MFI High	160	9.6
22	C - 30mm	K 90°	K 90°	C - 30mm	PP - MFI High	80	4.8

Exp No.	Element 1	Element 2	Element 3	Elment 4	Polymer	Screw Speed (rpm)	Feed Rate (kg/hr)
23	C - 30mm	K 90°	K 90°	C - 30mm	PP - MFI High	160	9.6
24	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI Mid	80	4.8
25	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI Low	80	4.8
26	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI Low	80	4.8
27	C - 30mm	C - 30mm	K 90°	K 90°	PP - MFI Low	80	4.8
28	C - 30mm	C - 30mm	K 90°	K 90°	PC	80	4.8
29	C - 30mm	C - 30mm	K 90°	K 90°	PA	80	4.8
30	C - 30mm	C - 30mm	K 90°	K 90°	PC	80	4.8
35	K 60°	K 60°	K 90°	RC - 20mm	PP - MFI High	80	4.8
Key:	**C = conveying element; K = kneading element;** **RC = reverse conveying element**						

Table 3-1-1 – Screw element combinations used in single polymer trials

Firstly, two different combinations of elements were run over a range of outputs and screw speeds. This covered experiment numbers, 2 through to 13, and were tested initially to generate information for the software characterisation. Experiments 2 to 8 were with one configuration having kneading blocks within the Pept window, and experiments 9 to 13 had conveying elements within the Pept window. Both of these sets of data covered a range of outputs and screw speeds that enabled a picture to be produced of how the running conditions influenced residence time through the elements.

The next pair of experiments (14 & 15), were conducted both to validate the software being written at Eindhoven University, and to incorporate findings into the Ludovic software and Ximex. For this purpose the elements being studied needed to be full, so a 20 pitch reversing element was situated downstream to ensure a full section existed under the Pept window. In excess of 100 runs were conducted for each screw configuration in order to give sufficient data to enable statistical analysis on the results and to minimise the effect of any faulty readings.

Experiment numbers 16 to 19 were aimed at making a comparison between the 15 pitch and the 30 pitch conveying element at two different running conditions. The element under investigation was followed by two 90° kneading blocks which should ensure that the conveying element was full, or at least nearly full.

The original trial configurations, for experiments 2 to 8, had included a 30° kneading block, but, with the Pept window not being able to cover as wide a view as had been hoped, it meant that we had no data on 30° kneading blocks. The next two trials (20 & 21) were therefore included to add data for 30° blocks, and to enable a comparison to be made with 90° blocks from experiment numbers 16 & 17.

The issue of a limited Pept window was of concern to the consortium as it restricted our ability to study the whole process. It was therefore decided to see if shifting the screw profile along would enable us to visualise a longer length of screw. Experiments 22 & 23 are in fact the same as experiments 16 & 17, but with the screw profile shifted along by one 30mm element. Hence if element two in experiment 22 had the same characteristics as element three in experiment 16 then there would be a suggestion that a longer length could be examined by this technique. Unfortunately, because of the time taken in manipulating the vast amounts of data generated, and designing a suitable spreadsheet template for examining the data, there was not enough time left in the project to examine this approach and then to act upon the idea.

The two columns highlighted in table 3-1-1 indicate elements 2 and 3 which are fully within the Pept window. Only the last portion of element 1, and the first portion of element 4, can be observed by Pept. Most of the experiments were conducted in pairs, which are highlighted in the same colour. However, each experiment can be looked upon as two different studies; for instance experiment 19 looks at a 15 pitch conveying element at position 2, but it also looks at a 90° kneading block in position 3. We can also count the first situation as a 15p followed by a 90°kb, and the second as a 90°kb followed by a 90°kb.

Experiments 24-30 were carried out to investigate the influence of polymer viscosity and polymer type on flow through conveying and kneading elements by changing polymer type and temperature.

Experiment 35 was carried out to investigate the behaviour during melting (melt zone moved to modified barrel section by reducing upstream temperature and removing upstream kneading elements).

3.2 General remarks

All experiments for the study of the influence of different processing conditions on the residence times were carried out using the same PP-Polymer with an MFI of 70. This comparably low viscosity polymer was chosen to minimise the stress on the PEPT-Particle.

The temperature profile in the extruder was set to 220-240°C.

The screw setup of the upstream elements was kept constant as well to guarantee constant and comparable melt quality. The screw setup of the upstream elements was chosen to plasticise the polymer gently without to much shear stress in order to apply as less as possible stress to the PEPT-particle.

For the interpretation of especially the residence time graphs it is important to note the numbering of the elements underneath the PEPT-window as illustrated in figure 3-2-1. In the discussion of the residence time only the elements fully covered by the PEPT-window (element 2 and 3) are discussed.

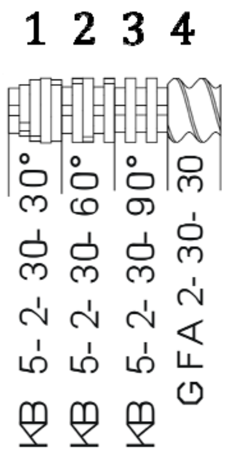


Figure 3-2-1: Numbering of the screw elements under the PEPTWindow

3.3 Effect of throughput on residence times

The following two chapters describe the effect of changing the throughput rate on the residence time and the residence time distribution when other processing conditions such as screw speed are kept constant.

3.3.1 Effect in Kneading discs

The following section discusses the influence of different processing conditions on standard kneading discs. For this study a kneading disc section with 60° and 90° kneading discs was configured under the PEPT-window.

3.3.1.1 Screw Configuration

A screw setup with a 60° and a 90° kneading disc was chosen for this study. A 30° kneading disc was in front of this setup, which was followed by a simple 30 mm pitch conveying element. The whole setup is illustrated in Figure 3-3-1

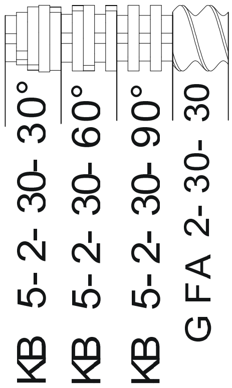


Figure 3-3-1: Screw setup for experiments 5 and 6

3.3.1.2 Processing conditions

For the study of the effect of throughput on the residence time and the residence time distribution two different processing conditions were chosen:

	Experiment 5	Experiment 6
Temperature, °C	220-240	220-240
Screw speed, 1/min	200	200
Feedrate, kg/h	4.8	9.6

3.3.1.3 Effect on residence time

The effect on the residence time distribution of the change in processing conditions between experiments 5 and 6 is illustrated in the three following graphs 3-3-2, 3-3-3 and 3-3-4

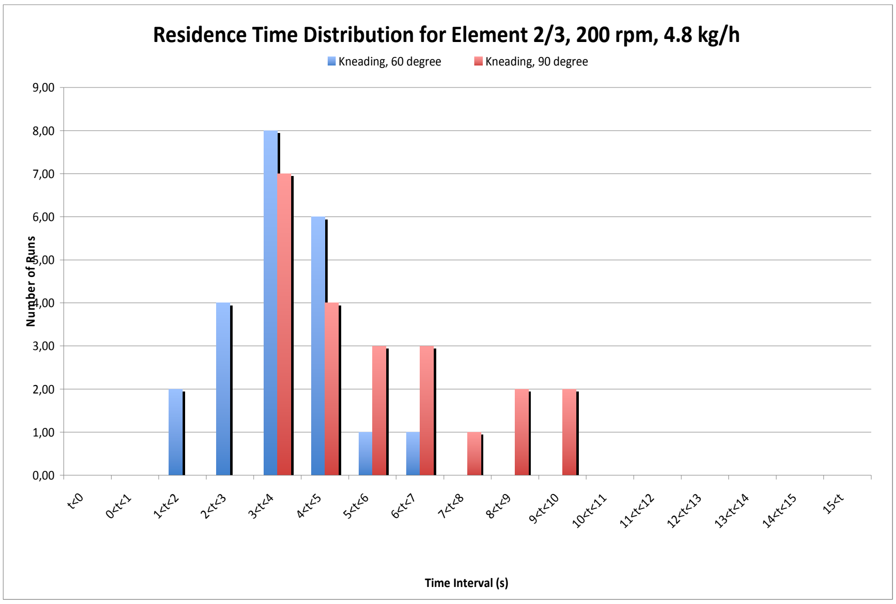


Figure 3-3-2: residence time distribution for 4.8 kg/h

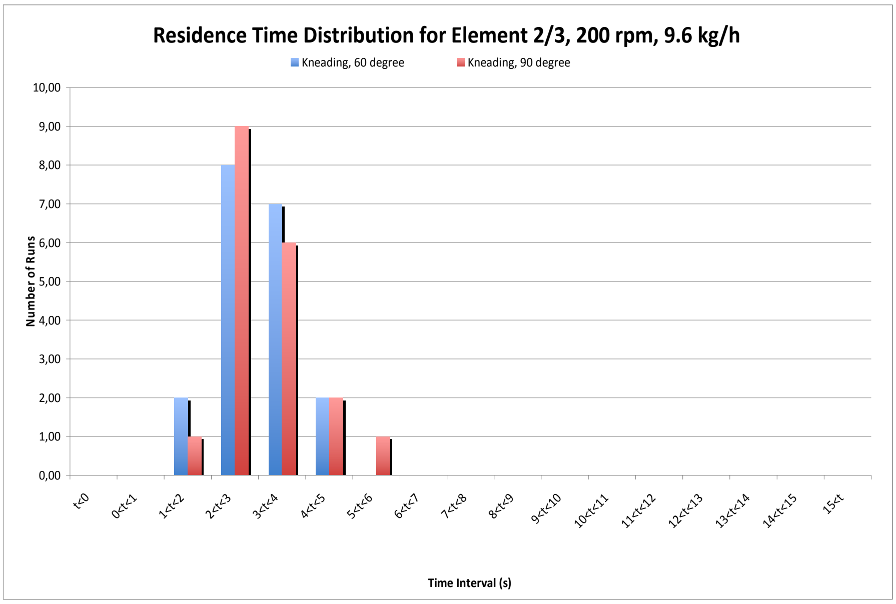


Figure 3-3-3: residence time distribution for 9.6 kg/h

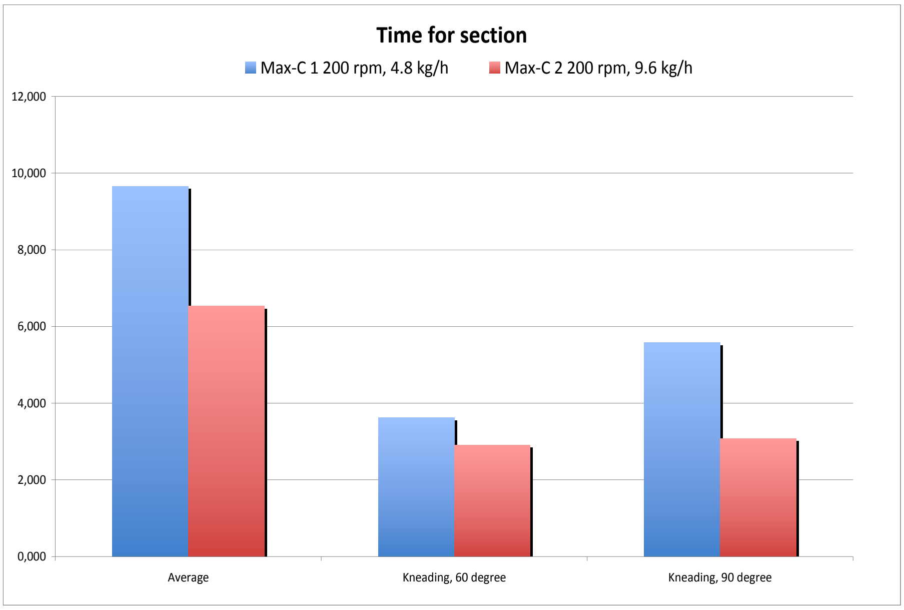


Figure 3-3-4: average residence time for 4.8 and 9-6 kg/h

The change in throughput from 4.8 to 9.6 kg/h while keeping the other processing conditions constant has a quite substantial effect on the residence time distribution. Figure 3-3-2 and 3-3-3 clearly shows a different residence time distribution for the two elements, which is also reflected in the average residence times shown in figure 3-3-4. The 60° kneading disc shows a narrower distribution and a shorter average residence time at 4.8 kg/h then the 90° kneading disc. The fill level can explain this large difference in residence time for these two kneading discs. The 60° kneading disc has a small but positive conveying capacity. At such a low throughput this results in the 60° kneading disc not being 100% full.

At 9.6 kg/h the situation changes quite substantially. The average residence time for the 60° discs is reduced by about 25%, whereas the 90° disc shows around a 50% residence time reduction. The later was expected because of the fully filled state, where the material flow is a direct function of the material volume flow through the screw geometry. Most interestingly the situation in the 60° kneading disc changes completely and the average residence time as well as the residence time distribution is now very similar to the 90° kneading disc. This can be explained by the 60° element now being fully filled and therefore the residence time is only a function of the material flow, which is now identical in both elements.

It is important to note that this was not expected to this extent. The change in throughput narrowed the residence time distribution for both kneading discs. This clearly reflects a decrease in distributive mixing efficiency of kneading discs at higher output rates or degree of fill.

3.3.1.4 Summary

Higher throughput in a kneading disc section results in:

- shorter residence time
- narrowed residence time distribution
- increase in fill level from partially filled to 100% filled for non-90° kneading discs.

3.3.2 Effect in conveying elements

After looking in detail on the effect of throughput on residence time distribution in kneading disc, the following section describes the effect of changing the throughput in conveying section.

3.3.2.1 Screw Configuration

A screw setup with a 40mm and a 30mm conveying element was chosen for this study. A 40mm conveying element was in front of this setup, which was followed by a simple 30 mm pitch-conveying element. The whole setup is illustrated in figure 3-3-5

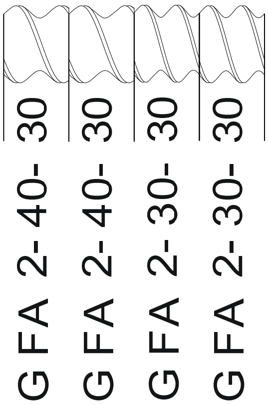


Figure 3-3-5: Screw setup for experiment 9 and 12

3.3.2.2 Processing conditions

For the study of the effect of throughput on the residence time and the residence time distribution two different processing conditions were chosen:

	Experiment 9	Experiment 12
Temperature, °C	220-240	220-240
Screw speed, 1/min	80	80
Feedrate, kg/h	4.8	9.6

3.3.2.3 Effect on residence time

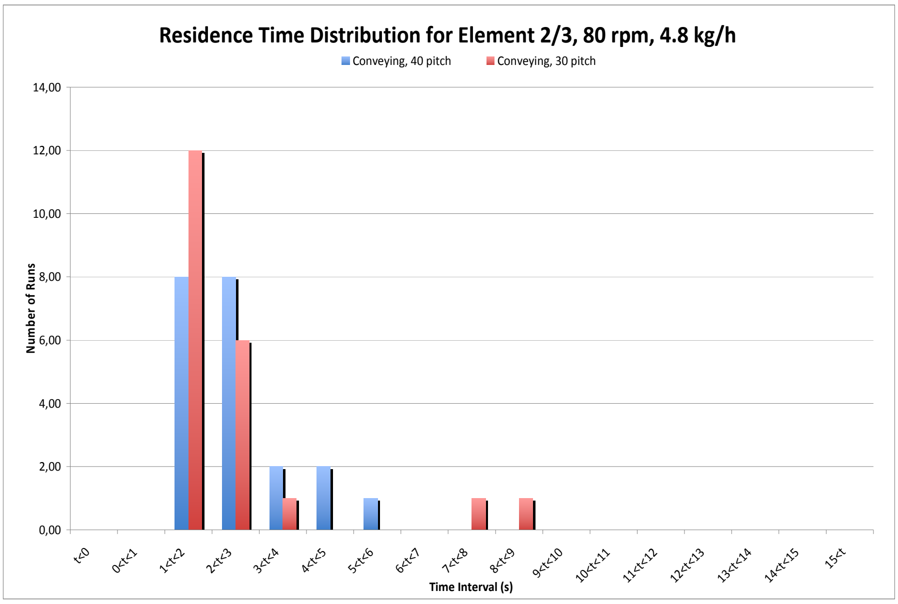


Figure 3-3-6: residence time distribution for 4.8 kg/h

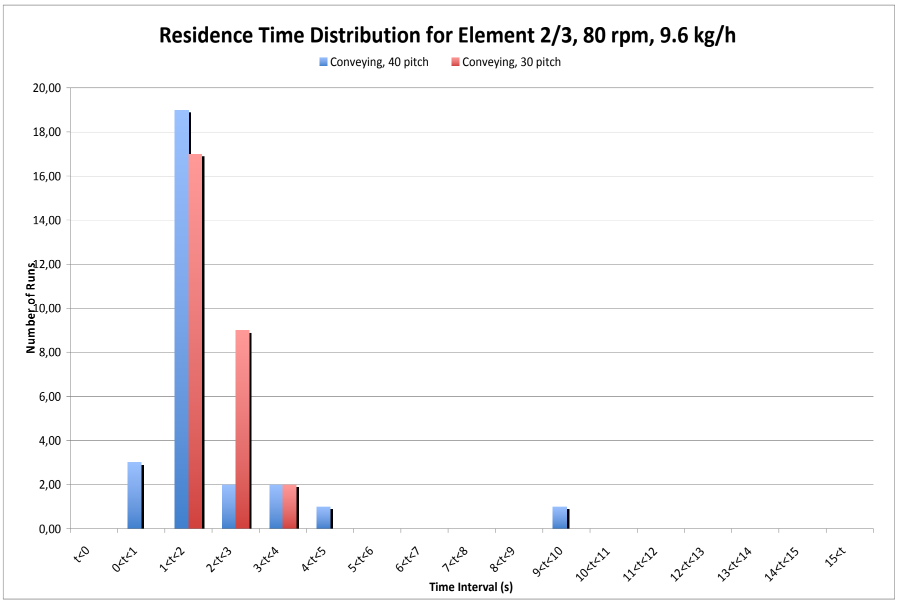


Figure 3-3-7: residence time distribution for 9.6 kg/h

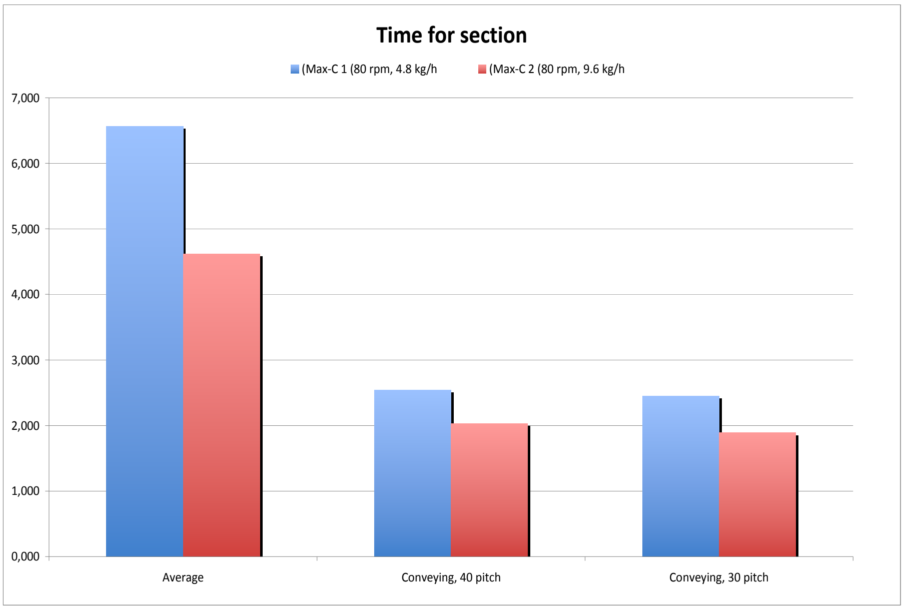


Figure 3-3-8: average residence time for 4.8 and 9-6 kg/h

By comparing the effect of changing the throughput in a conveying section to the effect the same change in processing conditions has in a kneading disc section, it is firstly obvious that the average residence time for the conveying section is significantly shorter and the residence time distribution is a lot narrower for the conveying elements. There are some quite slow passages, as can be seen in figures 3-3-6 and 3-3-7, but the residence time distribution for both conditions shows a sharp peak and short passage times. In absolute values, for the 90° kneading disc compared to the conveying elements, the average residence time is less than 50% for the conveying element.

Looking on the effect of changing the throughput for the conveying element section, it can be noted that the average residence time, as well as the shape of the residence time distribution, does not change significantly by increasing the throughput from 4.8 kg/h to 9.6 kg/h. The explanation for this is that the elements are not 100% full for the 4.8 kg/h condition and most probably also for the 9.6 kg/h condition. Therefore there is enough conveying capacity left to take up the additional material. Interestingly, the average residence time decreases for the conveying element when the throughput is increased, although these elements are not 100% full. Looking at the shape of the residence time distribution and taking into account that the peak passage times is between 1 and 2 seconds for both conditions, then this perhaps not directly anticipated phenomena can mainly be explained by a significant reduction in long passages for the higher throughputs.

3.3.2.4 Summary

Effect of changing the throughput in a conveying element section:

- As long as the element is conveying:
  → The effect on the residence time distribution is minor
- Small shift towards smaller residence time

3.4 Effect of screw-speed on residence times

Screw speed is an important factor in running compounding processes. As rotating twin screw extruders are mainly run in starve feed mode, screw speed has no effect on the throughput of the machine. Screw speed mainly influences the residence time in the conveying sections and varies the amount of shear and mixing efficiency in the kneading sections.

3.4.1 Effect in Kneading discs

3.4.1.1 Screw Configuration

A screw setup with a 60° and a 90° kneading disc was chosen for this study. A 30° kneading disc was in front of this setup, which was followed by a simple 30 mm pitch conveying element. The whole setup is illustrated in Figure 3-4-1.

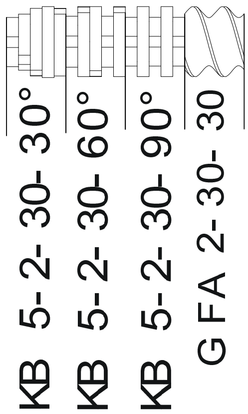


Figure 3-4-1: Screw setup for experiments 5 and 7

3.4.1.2 Processing conditions

For the study of the effect of screw speed on the residence time and the residence time distribution two different processing conditions were chosen:

	Experiment 5	Experiment 7
Temperature, °C	220-240	220-240
Screw speed, 1/min	120	200
Feedrate, kg/h	9.6	9.6

3.4.1.3 Effect on residence time

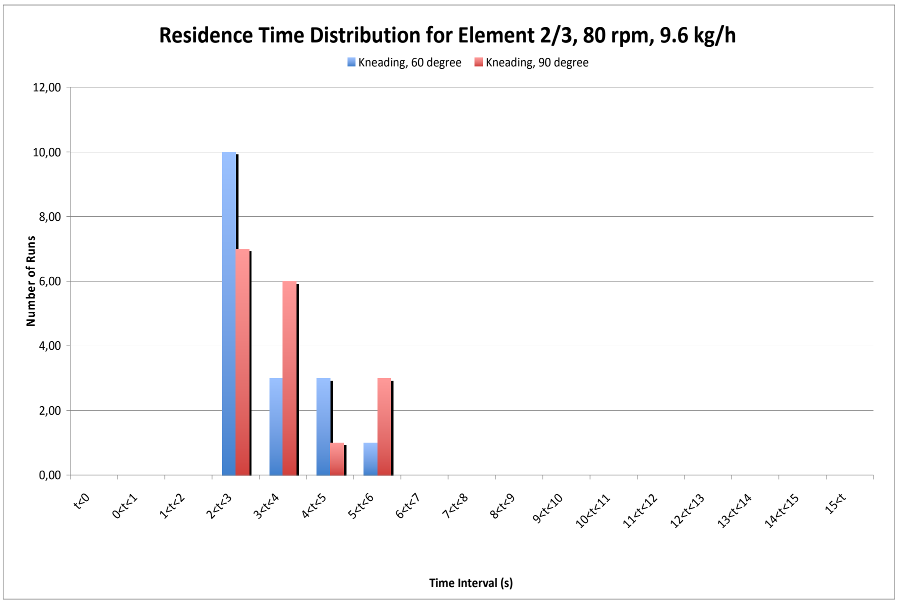


Figure 3-4-2: residence time distribution for 80 rpm

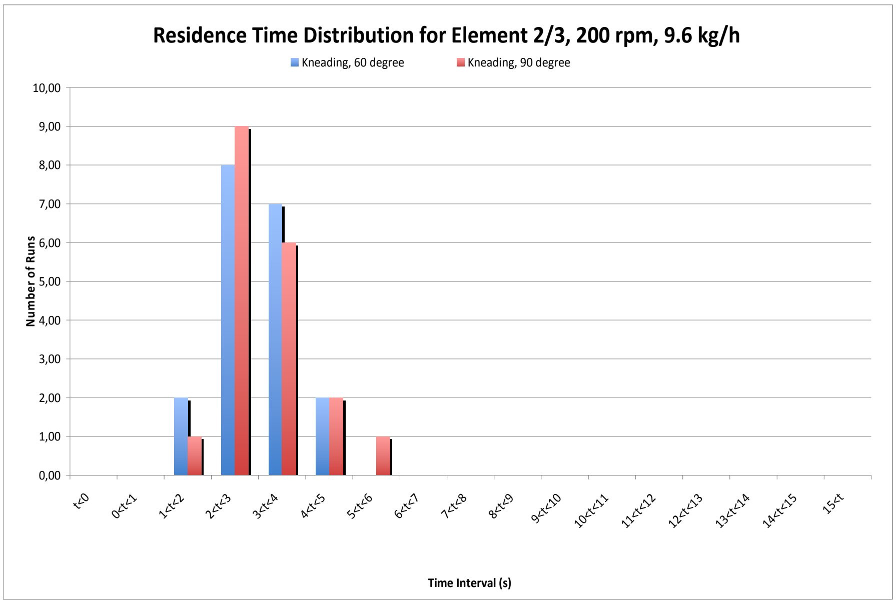


Figure 3-4-3: residence time distribution for 200 rpm

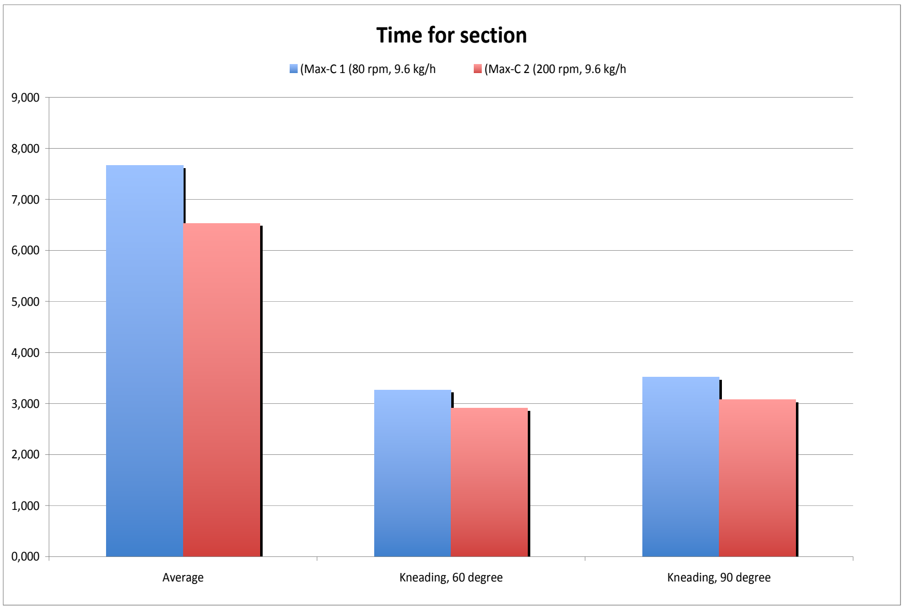


Figure 3-4-4: residence time distribution in comparision

In a kneading disc section, especially in those with larger staggering angle, it can be assumed they are fully filled, due to the very limited conveying capacity. Material flow and consequently the residence time and the residence time distribution can be expected to be mainly a function of the material volume flow in these sections, mostly independent from the processing parameters.

PEPTFlow results confirm this expectation. Although the shape of the residence time distribution illustrated for the two conditions (80 and 200 rpm) in figures 3-4-2 and 3-4-3 show differences, the average residence times illustrated for elements 2 and 3 in figure 3-4-4 are very similar.

The low number of experimental runs used to generate the data can explain the differences in the shape of the residence time distribution.

3.4.2 Effect in conveying elements

3.4.2.1 Screw Configuration

A screw setup with a 40mm and a 30mm conveying element was chosen for this study. A 40mm conveying element was in front of this setup, which was followed by a simple 30 mm pitch-conveying element. The whole setup is illustrated in Figure 3-4-5

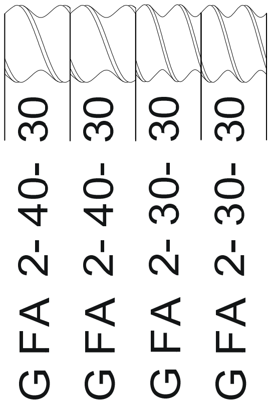


Figure 3-4-5: Screw setup for experiment 9 and 10

3.4.2.2 Processing conditions

For the study of the effect of screw speed on the residence time and the residence time distribution two different processing conditions were chosen:

	Experiment 9	Experiment 10
Temperature, °C	220-240	220-240
Screw speed, 1/min	80	200
Feedrate, kg/h	4.8	4.8

3.4.2.3 Effect on residence time

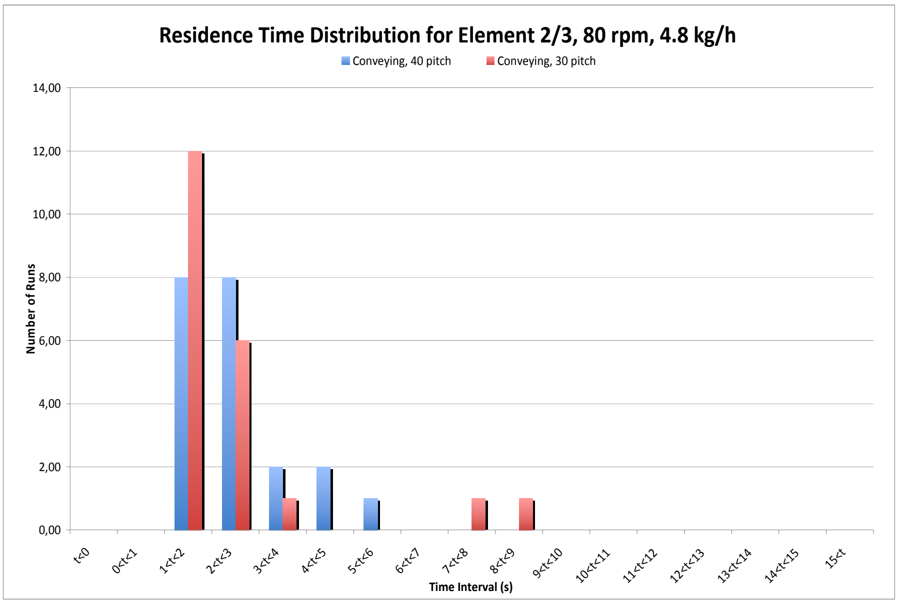


Figure 3-4-6: residence time distribution for 80 rpm

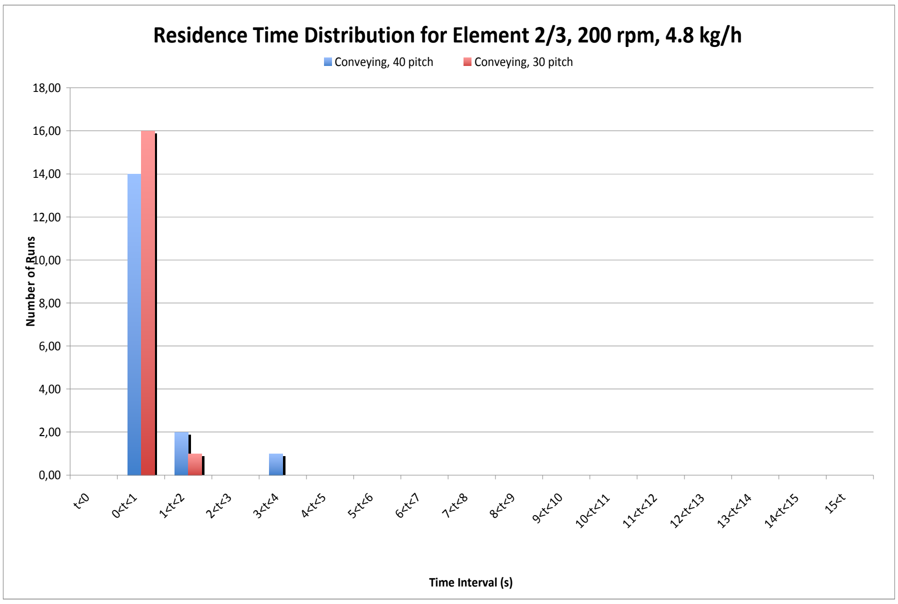


Figure 3-4-7: residence time distribution for 200 rpm

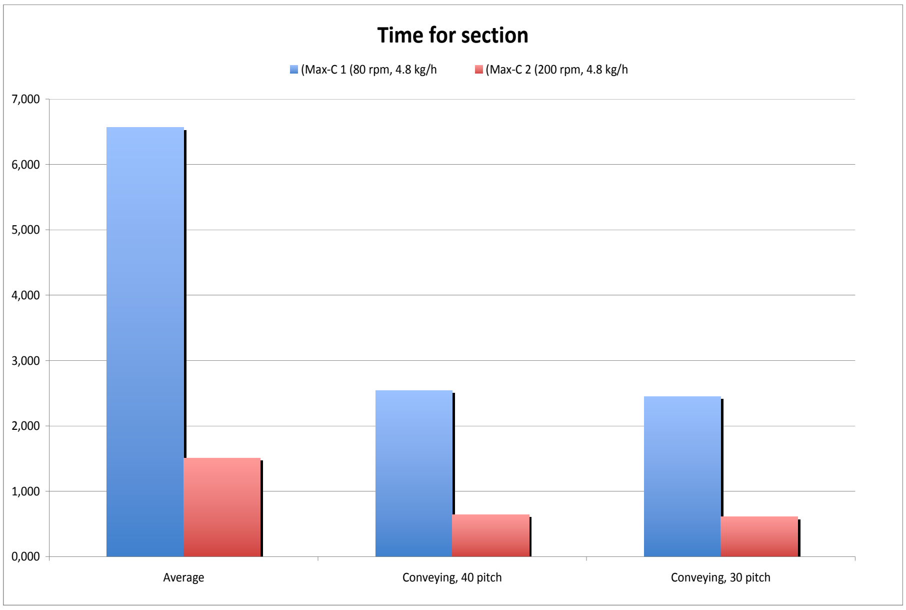


Figure 3-4-8: Comparison of average residence times

Conveying sections show a completely different processing behaviour than kneading discs. As long as those elements have enough conveying capacity to pump the material forward and as long as there is no substantial back pressure they are not fully filled and therefore the material flow is a direct function of the screw speed.

Figures 3-4-6 and 3-4-7 clearly confirm this for the two processing conditions 80 and 200 rpm.

By changing the screw speed from 80 to 200 rpm the residence time is reduced to almost 1/3 of the original residence time. Furthermore, the residence time distribution is narrowed drastically by increasing the screw speed. At 80 rpm the residence times of the passages varies from 1 to 9 seconds. At 200 rpm the residence times varies from 1 to 4 seconds with a sharp peak at times of 1 second.

3.4.2.4 Summary

Effect of changing the Screw Speed in a conveying element section:

- Strong shift towards smaller residence time
- Very narrow residence time distribution
- Narrowed down residence time distribution with higher rpm

3.5 Effect of the screw-fill on residence times

It is a common assumption that processing conditions are not drastically changed as long as one keeps the screw fill level constant. To illustrate that this common assumption that can often be heard from compounders is not true, this experiment was set up within the PEPTFlow experimental plan.

3.5.1 Effect in conveying elements and kneading discs

3.5.1.1 Screw Configuration

For this study the screw setup illustrated in figure 3-5-1 was used. Underneath the PEPT-Window are the second element (30mm pitch conveying element) and the third element (90° kneading disc). In front of the PEPT-window was a 30mm conveying element and the zone was followed by an additional 90° kneading disc.

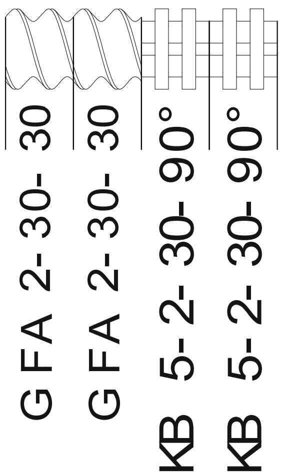


Figure 3-5-1: Screw setup for experiment 16 and 17

3.5.1.2 Processing conditions

For the study of the effect of screw fill on the residence time and the residence time distribution two different processing conditions were chosen:

	Experiment 16	Experiment 17
Temperature, °C	220-240	220-240
Screw speed, 1/min	80	160
Feedrate, kg/h	4.8	9.6

3.5.1.3 Effect on residence time

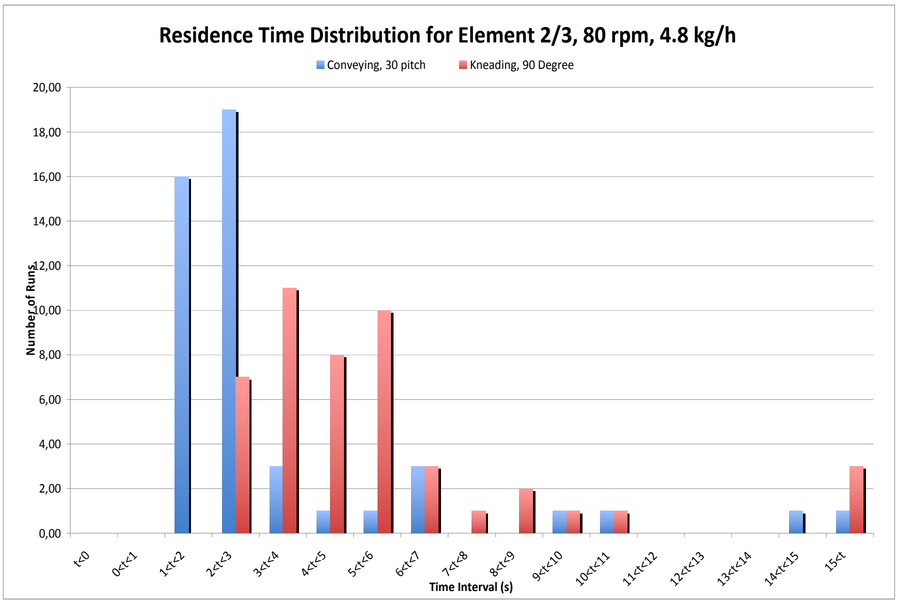


Figure 3-5-2: residence time distribution for 4.8 kg/h and 80 rpm

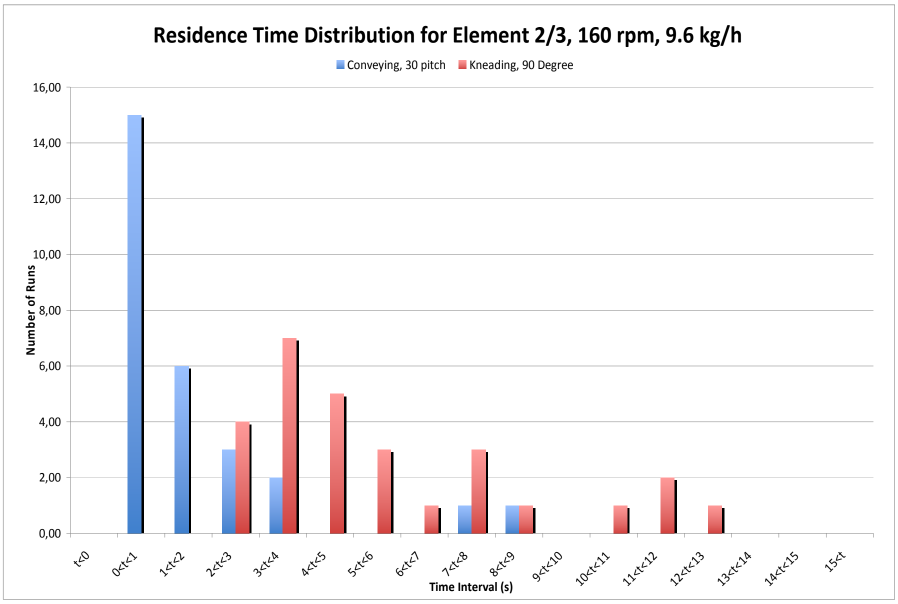


Figure 3-5-3: residence time distribution for 9.6 kg/h and 160 rpm

Changing the screw speed and proportionally changing the material throughput keeps the fill level constant in conveying elements as well as in kneading discs (which can be mostly considered as full).

In the conveying part of the observed screw configuration (blue graph) in figure 3-5-2 and 3-5-3 it can clearly be seen that the residence time distribution shifts towards smaller residence times with higher screw speeds at constant fill level.

In kneading disc sections the screw speed does not influence the residence time but does influence the mixing energy input. In these sections the material flow or feed rate influences the residence time.

3.5.1.4 Summary

The often-heard assumption that the processing does not change as long as one keeps the fill level constant does not prove to be correct.

Simultaneously changing rpm and throughput results in several changes to the processing conditions

- Higher rpm reduces residence time in conveying elements
- Higher throughput reduces residence time in kneading discs
- Constant fill levels at higher rpm reduce the residence time in the whole machine.
- In kneading disc sections the higher mixing intensity that goes along with the higher rpm is compensated for by the shorter residence time, so that at least the average mixing intensity can be assumed to be more or less constant by changing the processing according to the fill level.

3.6 Effect of back-pressure on residence times

3.6.1 Effect in conveying elements

3.6.1.1 Screw Configuration

For this study a screw setup was used, that contained a reverse element at the end of the PEPT-window section (here the 4th element). This element produces a strong backpressure guaranteeing that at least the conveying element in front of the reverse element is fully filled with melt. The reverse element has a pitch of only 20mm and the pressure build capacity of the reverse element is higher than the pressure build-up generated by the 30mm pitch conveying element in front of it. So it can be assumed that the fully filled section is also covering part of the second element underneath the PEPT-window (see figure 3-6-1).

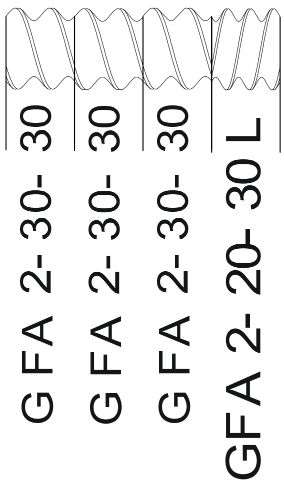


Figure 3-6-1: Screw setup for experiment 14

3.6.1.2 Processing conditions

For the study of the effect of backpressure on the residence time and the residence time distribution the following processing conditions were chosen:

	Experiment 14
Temperature, °C	220-240
Screw speed, 1/min	80
Feedrate, kg/h	4.8

PEPTFlow partner SCC has carried out a 3D simulation of this screw setup under the above processing conditions. The resulting melt pressure is illustrated in figure 3-6-2. It can be seen, that the pressure directly in front of the reverse element reaches almost 80 bars, with pressure of >40 bars going back at least one screw element.

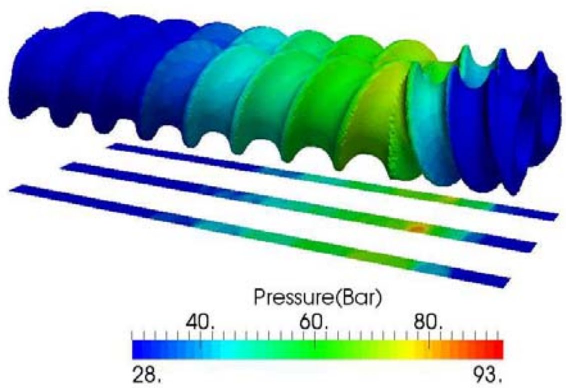


Figure 3-6-2: 3D simulation of the pressure in front of the reverse element.

3.6.1.3 Effect on residence time

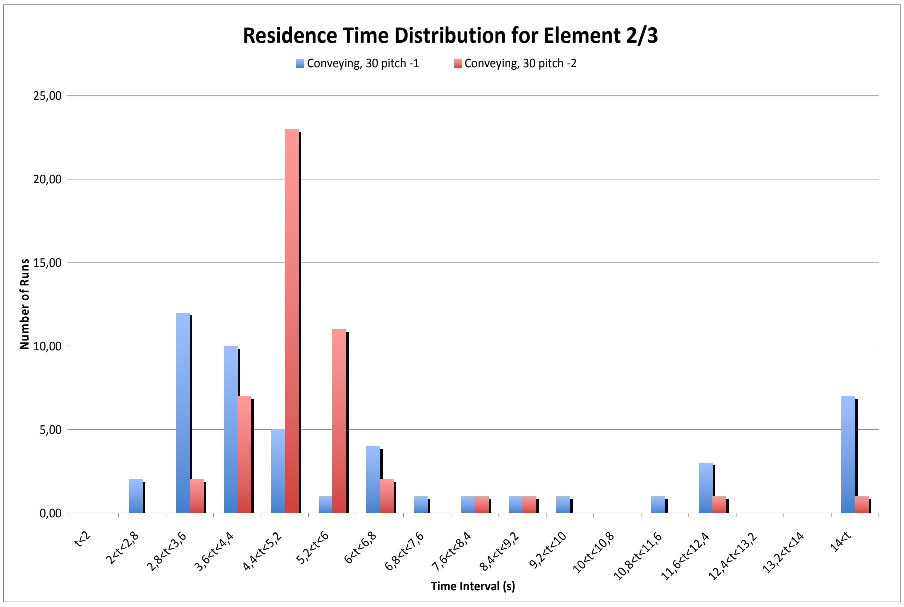


Figure 3-6-3: residence time distribution for element 2 and 3

Figure 3-6-3 illustrated substantial differences in the residence time and residence time distribution for the two monitored conveying elements underneath the PEPT-window. Element 2 can be assumed not to be fully filled, whereas element 3 can be regarded as being fully filled due to the backpressure.

The pressure level within the conveying elements has a very strong influence on the residence time distribution. Element 2, which is freely conveying the material in most of its length shows substantially shorter residence times than element 3. The peak of residence times shifts from 2.8-3.6 to 4.4-5.2 seconds by pressurising the conveying element with the reverse element. On the other hand the general shape of the main peak of the residence time distribution has not changed.

An important finding was made within the PEPTFlow-project concerning the influence of backpressure on the number of very long passage times or residence times. Looking on the right side of figure 3-6-3 it is very obvious, that the number of these long passages is reduced drastically in element 3, which has to build up pressure. This behaviour was not expected on first sight.

The most probable explanation of the reduction in long passages can be found if we consider the areas of the screws and barrels where these long residence times can happen. They mainly occur due to the melt film between the screw and barrel and on the screw surface. This melt film is not moving fast and has no substantial exchange with the main material stream.

Pressurising these section results in two phenomena, that consequently reduce the residence time:

- Due to the pressure build up the screws are a little bit more pushed towards the barrel. This reduces the clearance and consequently reduces the material stuck in the melt film
- Perhaps more important is that the backpressure increases the leakage flow over the screw tip and between the screws. This intensive material flow through these small gaps washes away the melt film, resulting in a much more intense exchange of the melt film with the main material flow.

3.6.2 Effect in Kneading discs

3.6.2.1 Screw Configuration

The following screw configuration was used for the trials with kneading discs in front of a reverse element to guarantee a 100% fill.

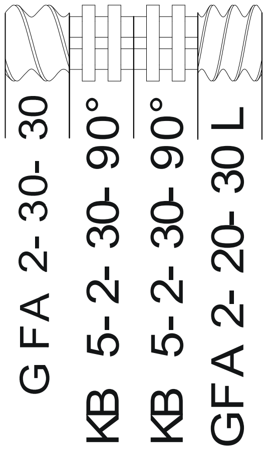


Figure 3-6-3: Screw setup for experiment 15

3.6.2.2 Processing conditions

	Experiment 15
Temperature, °C	220-240
Screw speed, 1/min	80
Feedrate, kg/h	4.8

PEPTFlow partner SCC has carried out a 3D simulation of this screw setup under the mentioned processing conditions. The resulting melt pressure is illustrated in figure 3-6-4. It can be seen, that the pressure directly in front of the first kneading disc element reaches almost 70 bars with a slight decrease towards the end of the kneading disc section and a steep decrease over the reverse element.

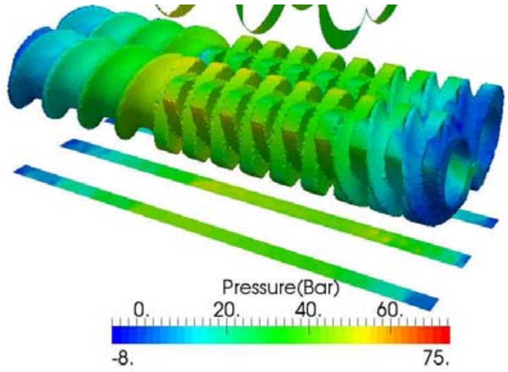


Figure 3-6-4: 3D simulation of the pressure in the screw profile

3.6.2.3 Effect on residence time

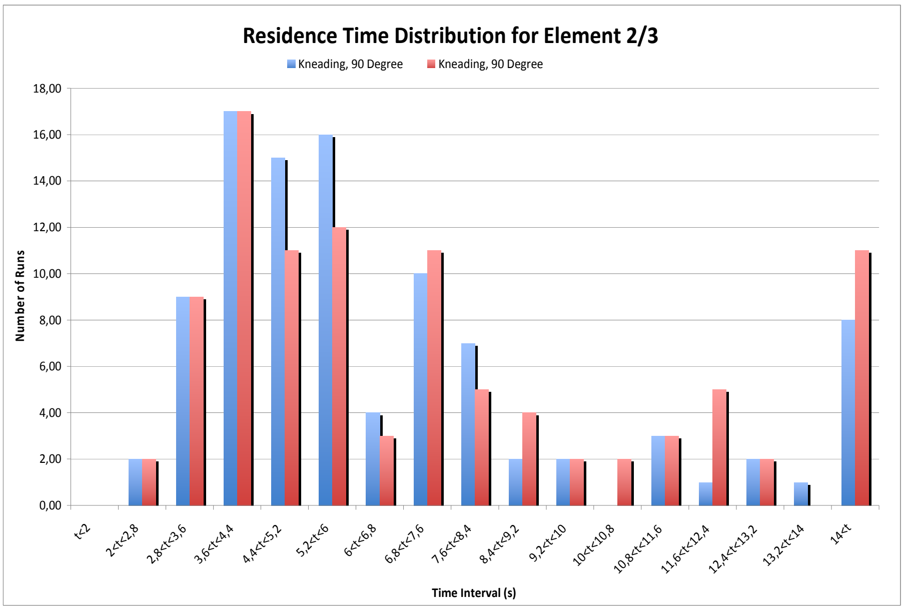


Figure 3-6-5: Residence time distribution for a 100% fully filled kneading disc section under backpressure.

In the kneading disc section that is fully filled under these processing conditions the effect of the pressure on the residence time and residence time distribution is negligible. This was assumed, as the backpressure only increases the static pressure in this area.

It should be noted, that there are a substantial amount of very slow passages that are summarised in the category 14plus seconds at the right side of the graph. They reflect the good axial mixing capacities of kneading discs but they can also be a problem with temperature sensitive materials.

3.6.2.4 Summary

The influence of backpressure can be summarised:

- Longer and broader residence time in conveying elements
- Practically no influence in kneading discs
- Reduced number of “very slow” passages for conveying elements

4 Comparing PEPTFlow results with Ludovic 1 D Simulation

4.1 Comparing PEPTFlow results with 1D Simulation results for Conveying Elements

4.1.1 Overview of the processing conditions

When running the twin screw compounder, there are two major degrees of control: feed rate and screw speed. These are independent of each other and each one will influence degree of fill, residence time, and shear rate, to a greater or lesser extent. Information on the way residence time changes with output and screw speed is available from published literature (ref.1) and it was therefore possible to compare the PeptFlow measurements with previous work.

It was also possible to model the screw profile, using the 'Ludovic' software, and obtain information regarding the predicted total residence time for the screw. Experiment numbers 9 to 13 and numbers 2 to 8 were examined in this way. This group of experiments were analysed first as they dealt with two different pitch conveying elements, which are the basic unit within the twin-screw extruder. Also, from the survey conducted earlier in the project, and reported in deliverable D2, both machine manufacturers and processors considered conveying elements to be an important part of the project. The same survey also identified running conditions as being at the top of the list that respondents to the questionnaire felt would benefit from a greater understanding. Hence, this analysis of different running conditions is aimed at generating a better understanding of both the elements themselves, and also how running conditions alter the performance of both conveying elements and kneading blocks.

The following tables, 4-1-1 and 4-1-2, give an overview of the data extracted from the summary spreadsheet for each experiment 09 to 13. The data was selected in order to observe comparisons between elements and running conditions that were felt to be important with respect to the conveying and mixing performance of the elements. Also included was a term that expressed the accuracy of the statistical data bearing in mind that the number of runs conducted for each experiment varied from as low as 22 up to a maximum of 77 for experiments 9 to 13. There was also a measure of the ratio of screw occupancy, which will be discussed later in the section headed ‘occupancy ratio’.

Element Tested	40 pitch conveying				
Experiment Number	9	10	11	12	13
Feed rate (kg/hr)	4.8	4.8	9.6	9.6	7.2
Screw speed (rpm)	80	200	200	80	140
Number of runs	22	23	37	30	77
Standard error	21.3%	20.9%	16.4%	18.3%	11.4%
Rt Mean (secs)	2.545	0.641	0.596	2.033	1.891
Rt Median (secs)	2.323	0.354	0.448	1.551	1.538
Rt Standard deviation	1.296	0.847	0.309	1.734	1.058
Rt Coefficient of Variation	0.51	1.32	0.52	0.85	0.56
XY/XYZ Mean	0.924	0.554	0.819	0.899	0.938
XY/XYZ Std deviation	0.038	0.301	0.146	0.032	0.030
XY/XYZ Coef. Of variation	0.041	0.543	0.178	0.036	0.032
Average velocity (mm/s)	87.9	139.9	197.8	87.0	138.2
Max acceleration (mm^2/s)k	148.5	11.8	70.6	72.4	89.3
Occupancy left/right	1.146	1.375	1.262	1.278	1.475
Pbs	1.381	0.588	0.700	1.750	1.885
Tip passes	3.571	0.235	0.700	3.464	2.574
Pbs + Tip passes	4.952	0.823	1.400	5.214	4.459
Ratio velocity>threshold	7.40%	0.90%	1.30%	22.40%	13.80%
% Tip passes	0.3%	0.0%	0.3%	0.5%	0.4%

Table 4-1-1 Data for 40 pitch conveying element (experiments 9 to 13)

Element Tested	30 pitch conveying				
Experiment Number	9	10	11	12	13
Feed rate (kg/hr)	4.8	4.8	9.6	9.6	7.2
Screw speed (rpm)	80	200	200	80	140
Number of runs	22	23	37	30	77
Standard error	21.3%	20.9%	16.4%	18.3%	11.4%
Rt Mean (secs)	2.452	0.612	0.634	1.889	1.533
Rt Median (secs)	1.763	0.522	0.479	1.659	1.358
Rt Standard deviation	1.978	0.367	0.389	0.69	0.848
Rt Coefficient of Variation	0.81	0.60	0.61	0.37	0.55
XY/XYZ Mean	0.902	0.733	0.803	0.896	0.926
XY/XYZ Std deviation	0.049	0.256	0.155	0.035	0.030
XY/XYZ Coef. Of variation	0.054	0.349	0.193	0.039	0.032
Average velocity (mm/s)	84.8	152.3	176.6	84.1	132.3
Max acceleration (mm^2/s)k	98.5	15.2	66.9	66.7	82.7
Occupancy left/right	0.988	1.967	1.028	0.919	1.320
Pbs	0.714	0.235	0.400	0.821	0.656
Tip passes	7.095	0.294	2.267	6.000	1.279
Pbs + Tip passes	7.809	0.529	2.667	6.821	1.935
Ratio velocity>threshold	7.20%	0.00%	9.80%	6.40%	13.40%
% Tip passes	0.9%	0.2%	0.7%	0.9%	0.2%

Table 4-1-2 Data for 30 pitch conveying element (experiments 9 to 13)

4.1.2 Residence Times

The following illustrations (Figures 4-1-1 to 4-1-6) show the screw profile, as modelled on the ‘Ludovic’ software supplied by project partner SCC. They show plots of melt temperature and local residence time for each of the five operating conditions used in experiments 09 to 13.

From these simulations it was possible to obtain the predicted total residence time for the whole screw and to plot contour lines for residence time on the graph of output vs screw speed, (Figure 4-1-7). This compares very well with published work (ref. 1) carried out in 1987/88 at ICI and Baker Perkins, on a 30mm twin-screw extruder, (Figure 4-1-8). This data helps to validate the Ludovic calculations as to how residence time changes with changes in operating conditions such as output and screw speed.

However, the Pept experiments were only able to measure the residence time of the particles as they travelled through elements two and three, shown earlier in figures 3-1-1 and 3-2-1, and not the whole screw. As mentioned previously, each experiment consisted of many runs, ranging from 22 to 77 for experiments 09 to 13. Each of these runs was loaded into a standard spreadsheet to enable calculations to be made regarding a wide range of items, which included residence time. Hence, for each experiment we were able to record an average, and a median residence time, plus a standard deviation for the residence time distribution that was obtained for that experiment. Within experiments 09 to 13 that meant that we were able to record this data for both of the conveying elements under test, 30 pitch, and 40 pitch, at each of the operating conditions studied.

The median residence times observed were then used to prepare a series of contour lines that were plotted on the graph of output (Q) vs screw speed (N). The Ludovic predictions (Figs. 4-1-2 to 4-1-6) were also treated in the same way and these contour lines plotted on the same graph for comparison. This was done for both the 30 pitch element and the 40 pitch element (Figures 4-1-9 and 4-1-10).

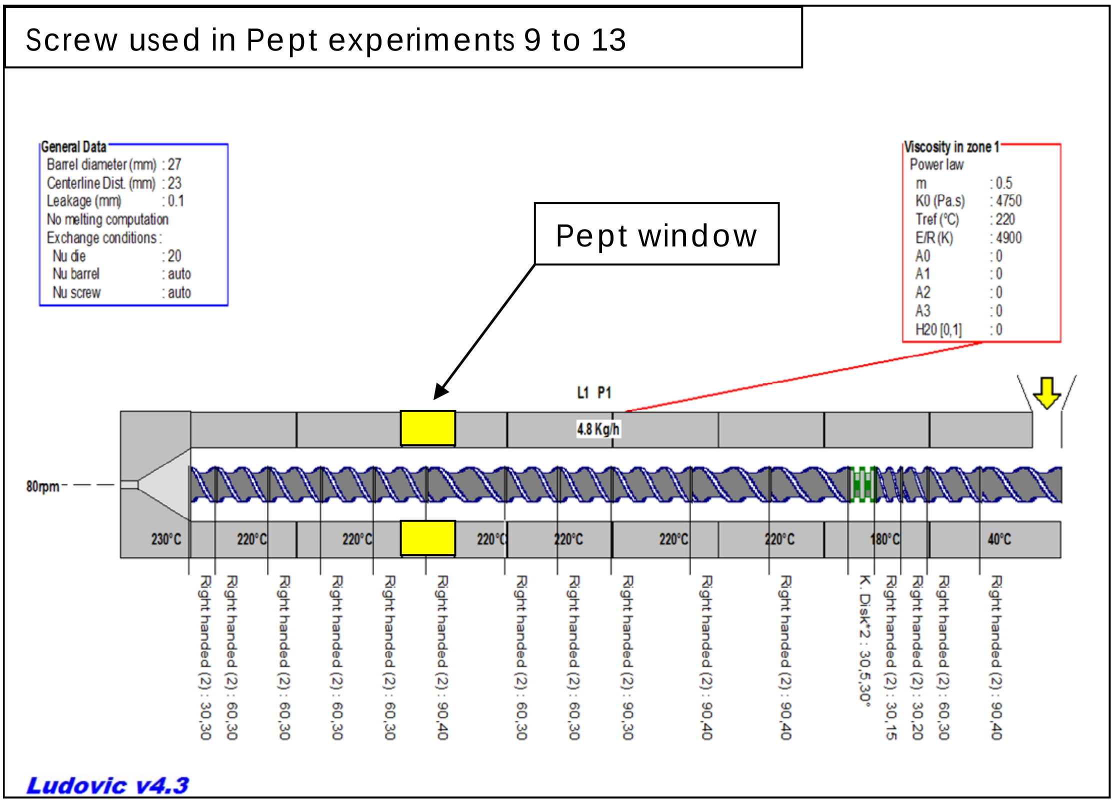


Figure 4-1-1 Screw used in Pept experiments 9 to 13 (Drawn in Ludovic).

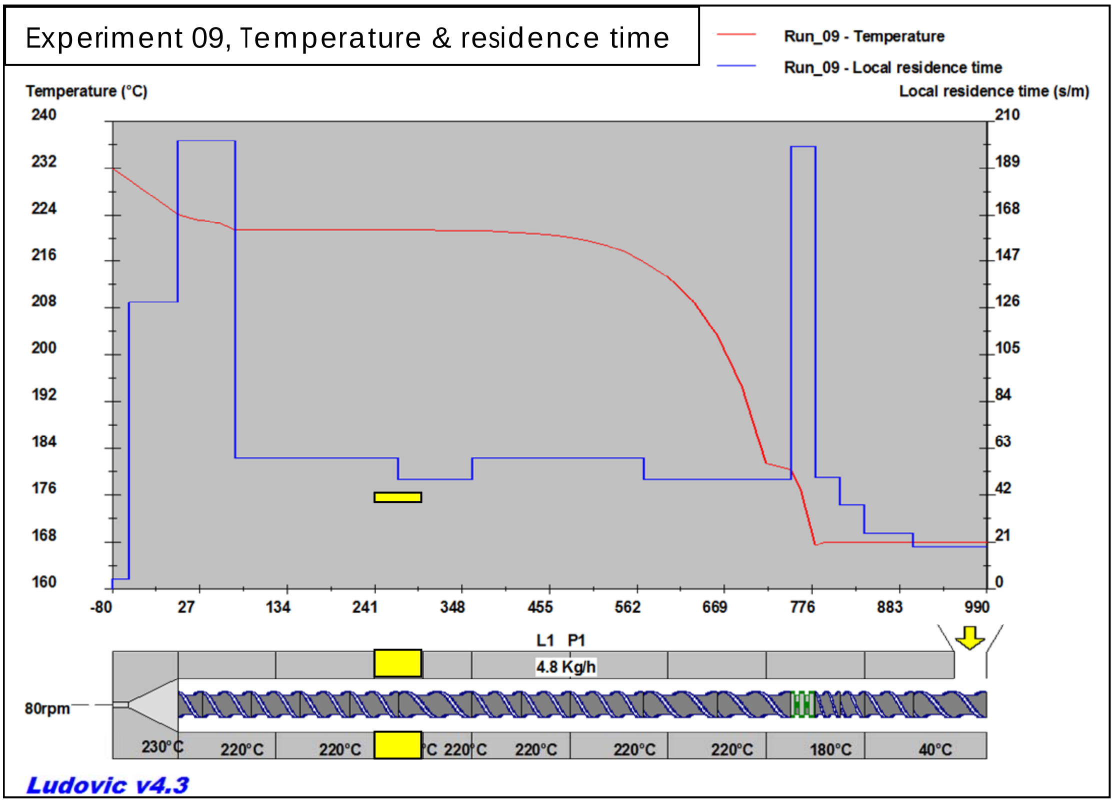


Figure 4-1-2. Ludovic predictions for experiment 09.

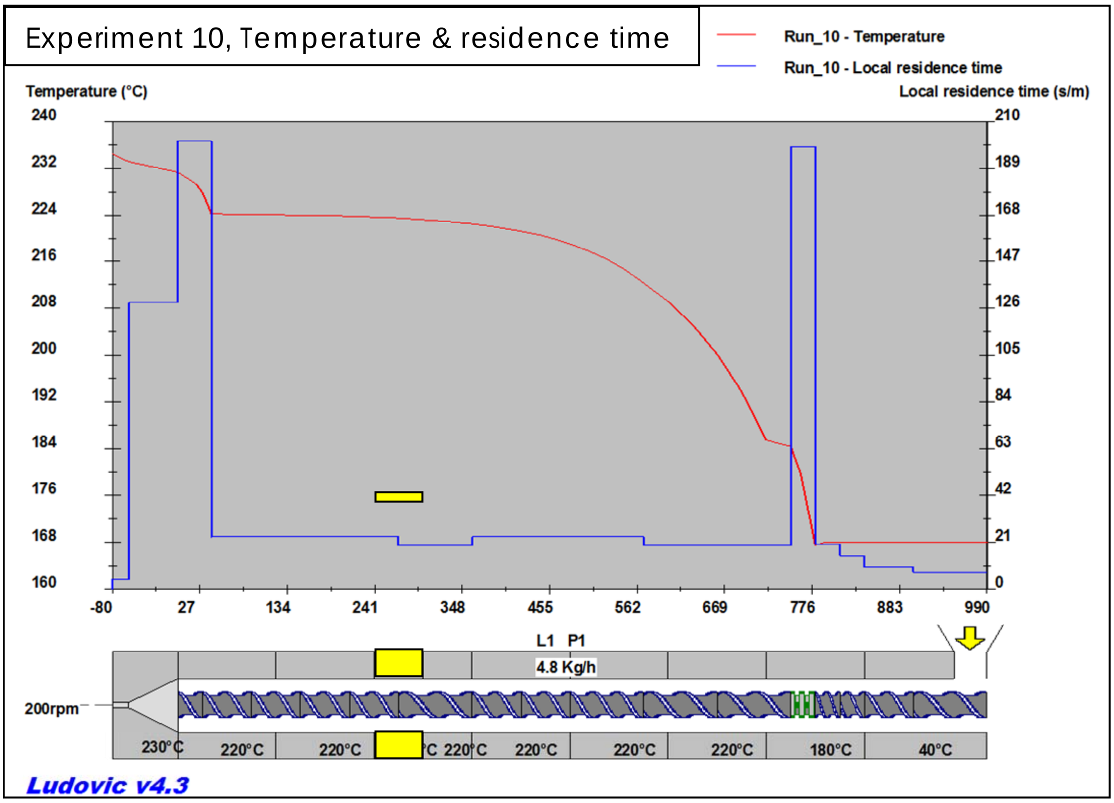


Figure 4-1-3 Ludovic predictions for experiment 10.

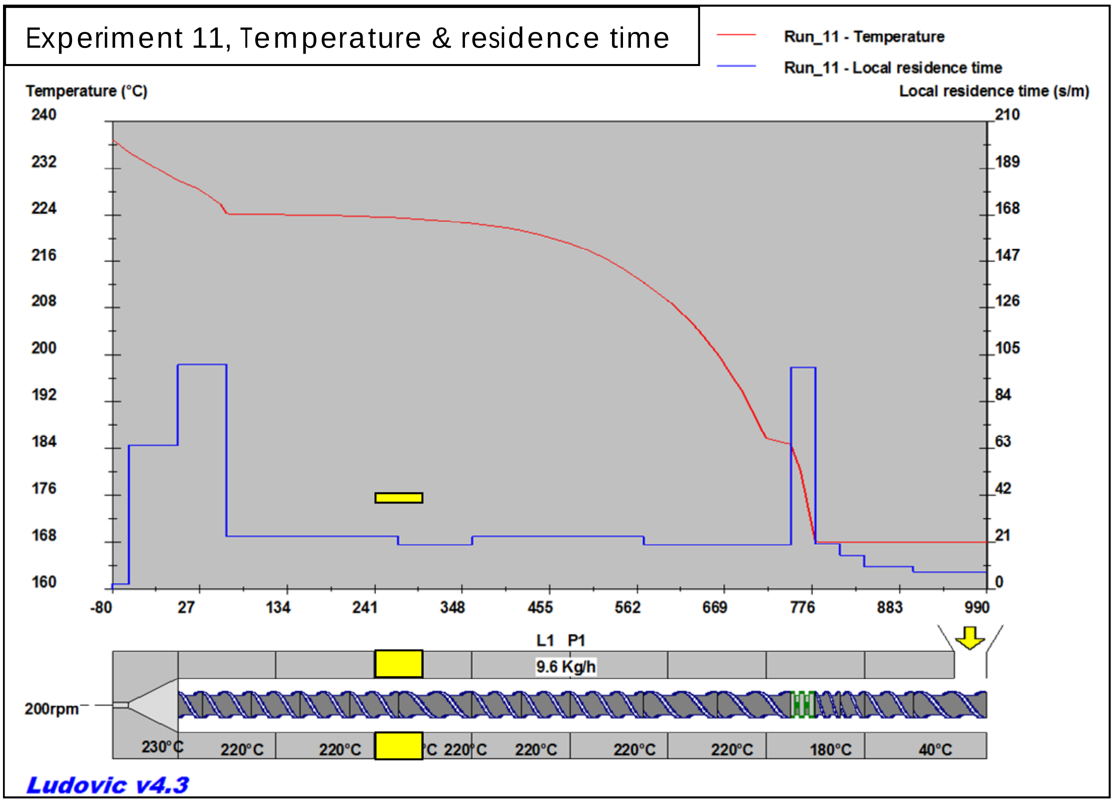


Figure 4-1-4 Ludovic predictions for experiment 11.

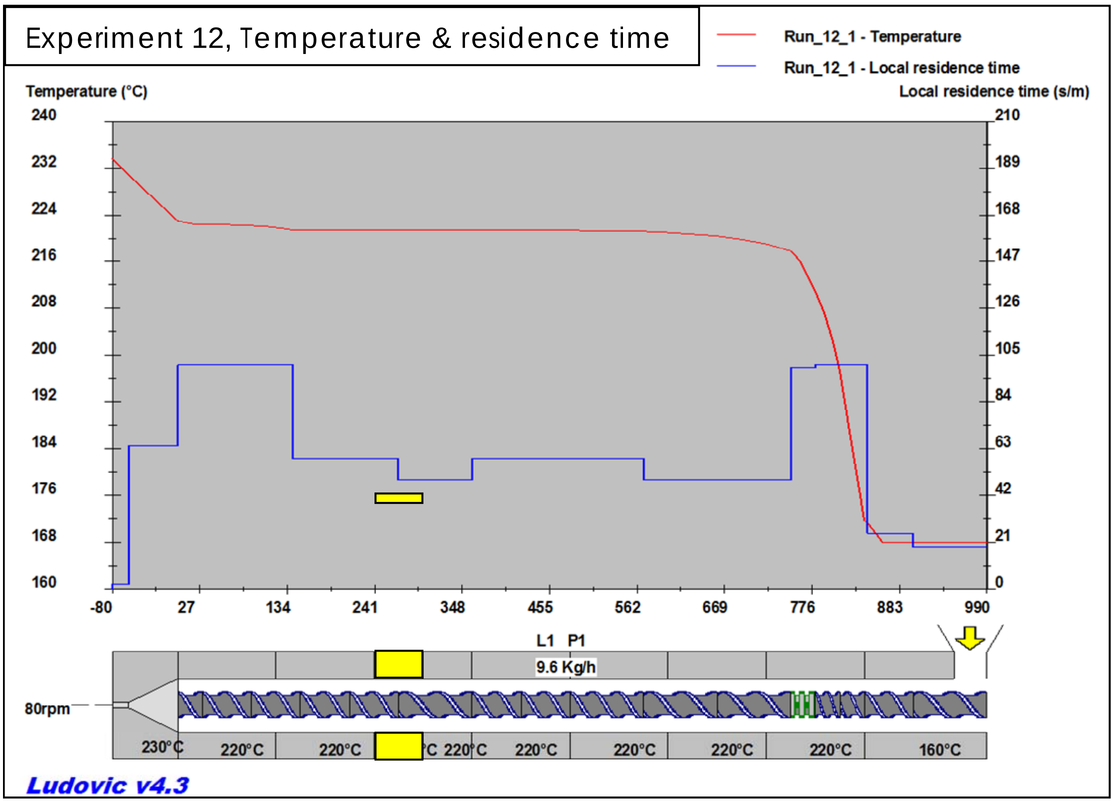


Figure 4-1-5 Ludovic predictions for experiment 12.

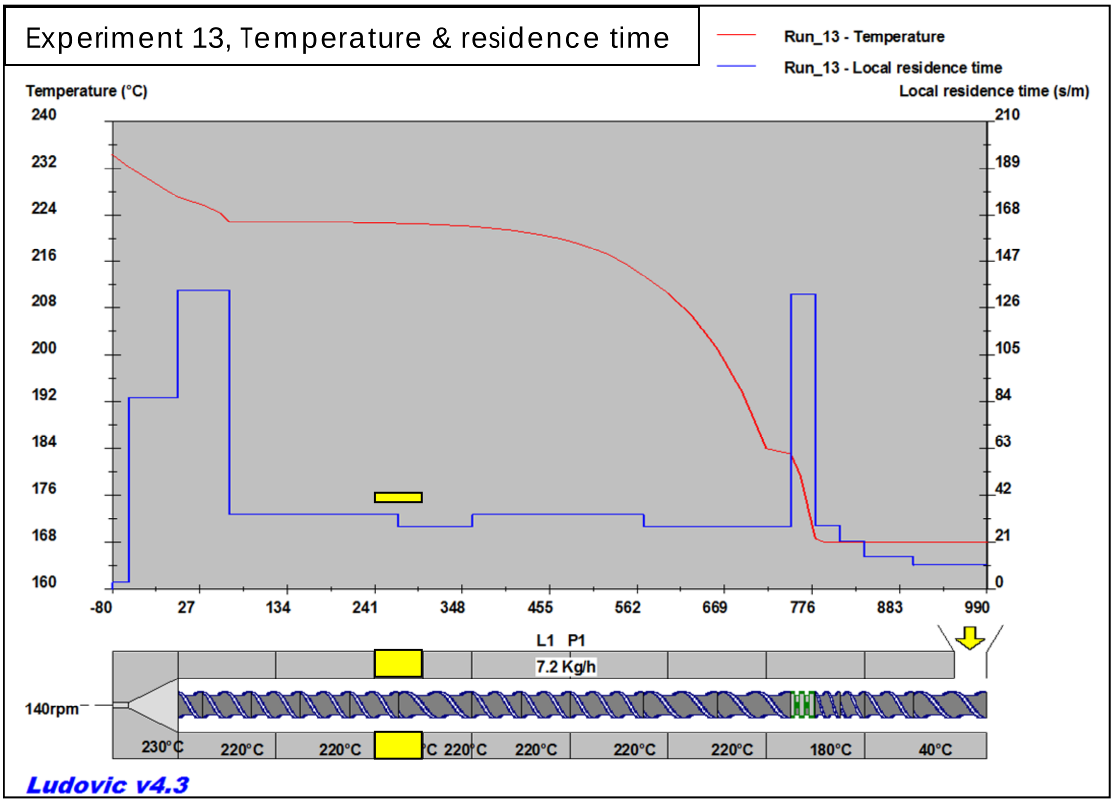


Figure 4-1-6 Ludovic predictions for experiment 13.

Figure 4-1-7 Ludovic Predictions for total residence time

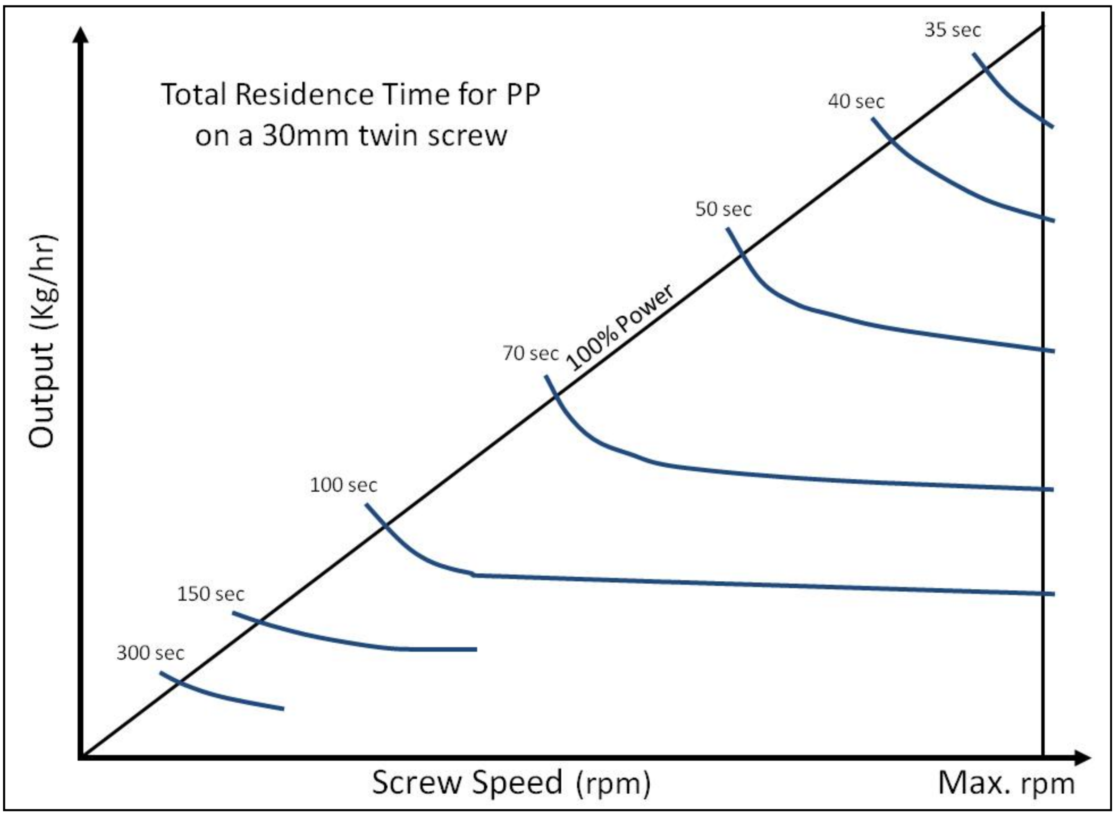


Figure 4-1-8 Q vs N, showing total residence time (from ref. 1)

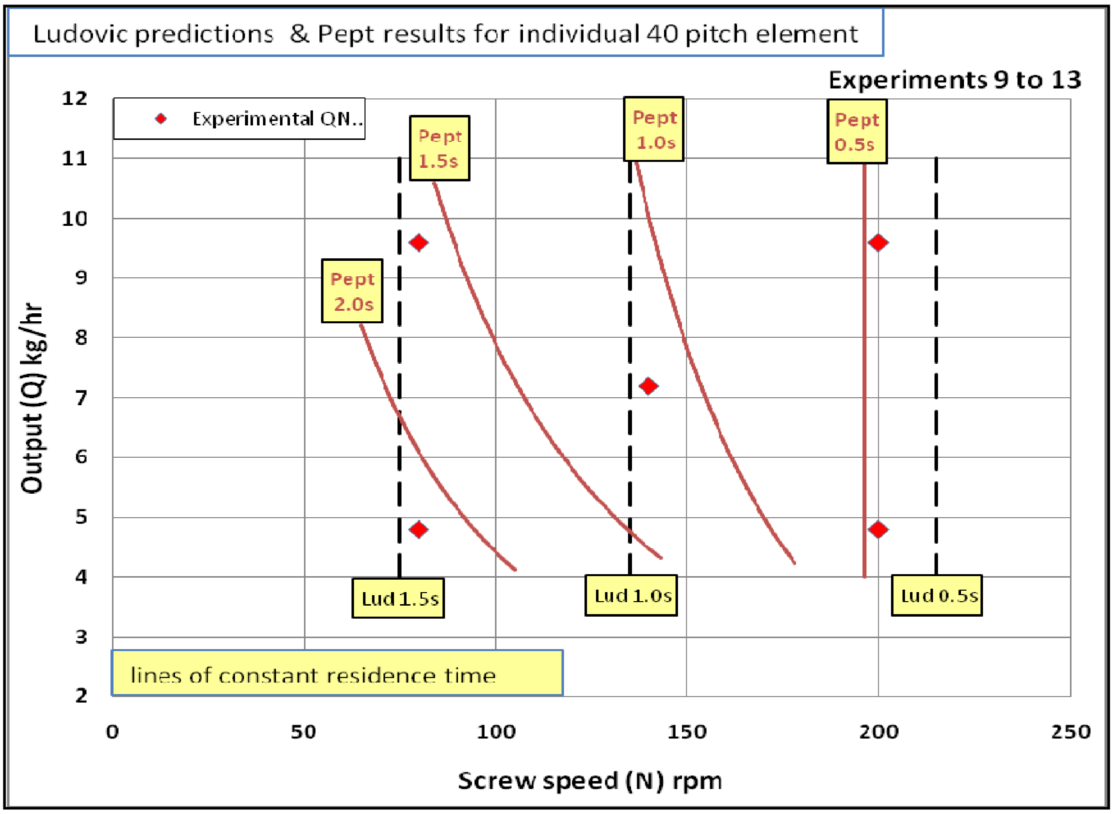


Figure 4-1-9 Residence times for 40 pitch conveying element

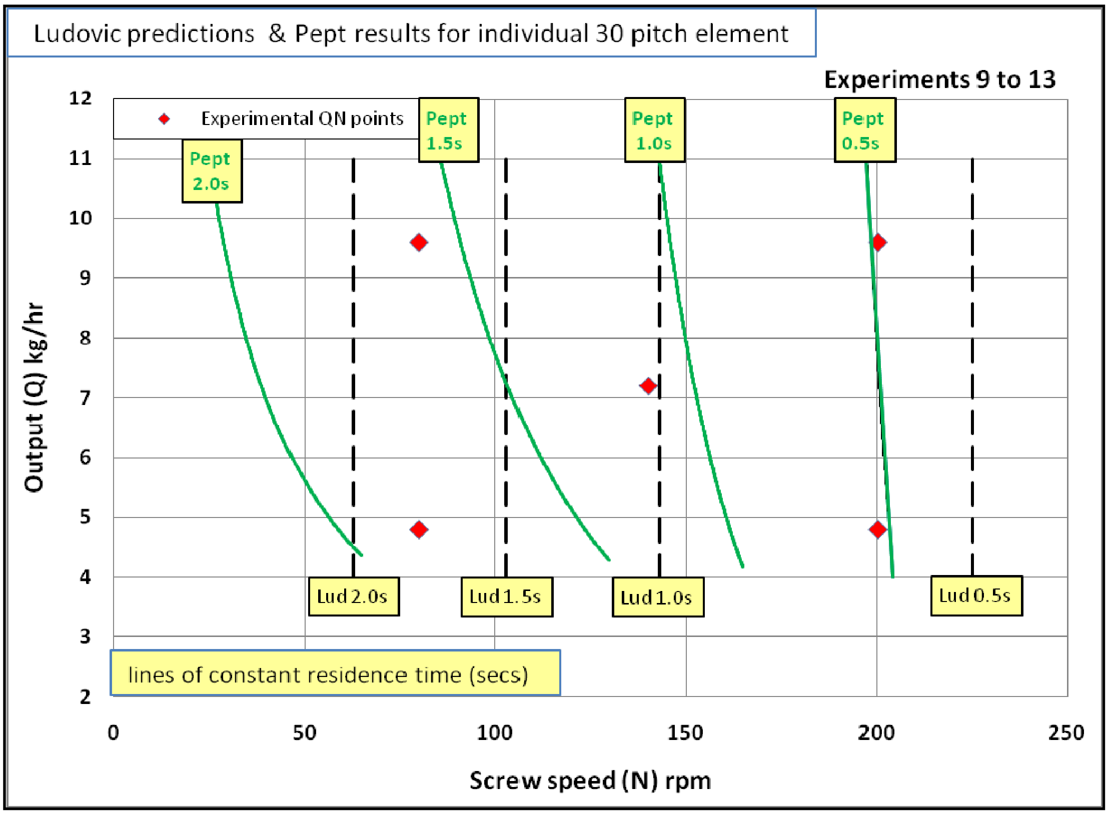


Figure 4-1-10 Residence times for 30 pitch conveying element

As can be seen from these illustrations the Ludovic predictions and the actual Pept measurements of residence time are very close to each other. This tends to verify both the Ludovic software, and the Pept technique, as they are either both wrong, or both right. However, from the earlier comparison of total residence time (Figs 4-1-7 and 4-1-8) it can be shown that the Ludovic predictions are very close to actual measurements conducted on the same size extruder 20 years previously. Hence, the conclusion must be that figures 4-1-9 and 4-1-10 are correct indications of the actual residence time and therefore the Pept experiments and the Ludovic predictions verify each other.

Occupancy Ratio

By monitoring the position of the particle, and recording which quadrant of the twin screw it was in at any one time, it was possible to measure how long the particle resided in the left hand screw and how long in the right when viewed from the discharge end of the extruder. Previous work at Baker Perkins, and general observations of open screw discharge, all point to a tendency for more material to be present on the left hand screw, viewed from the discharge of a clockwise rotating twin screw. This general industry view was actually confirmed by the PeptFlow results. The ratio of left/right hand screws varied from 0.919 up to 1.967 with only two out of the ten experiments (9 to 13) having a ratio of slightly less than one. What was even more interesting was the way in which this ratio changed with running conditions.

By plotting the experimental results on a graph of Output (Q) versus Screw Speed (N) it was possible to interpolate a rough idea of how the ratio varied. This information is shown in figures 4-1-11 and 4-1-12 below. There did appear to be a pattern emerging but we must remember that this was based upon just 5 different conditions. Further investigation of this effect would be of real interest, and could well influence screw design, but there was insufficient time left in the project to run further experiments that could have added to the knowledge. However, what can be concluded is that the PeptFlow results have confirmed an industry view regarding the distribution of the polymer between the two screws. It has also supplied enough data to warrant further investigation in the future, and shown that the Pept technique can be used for this type of study.

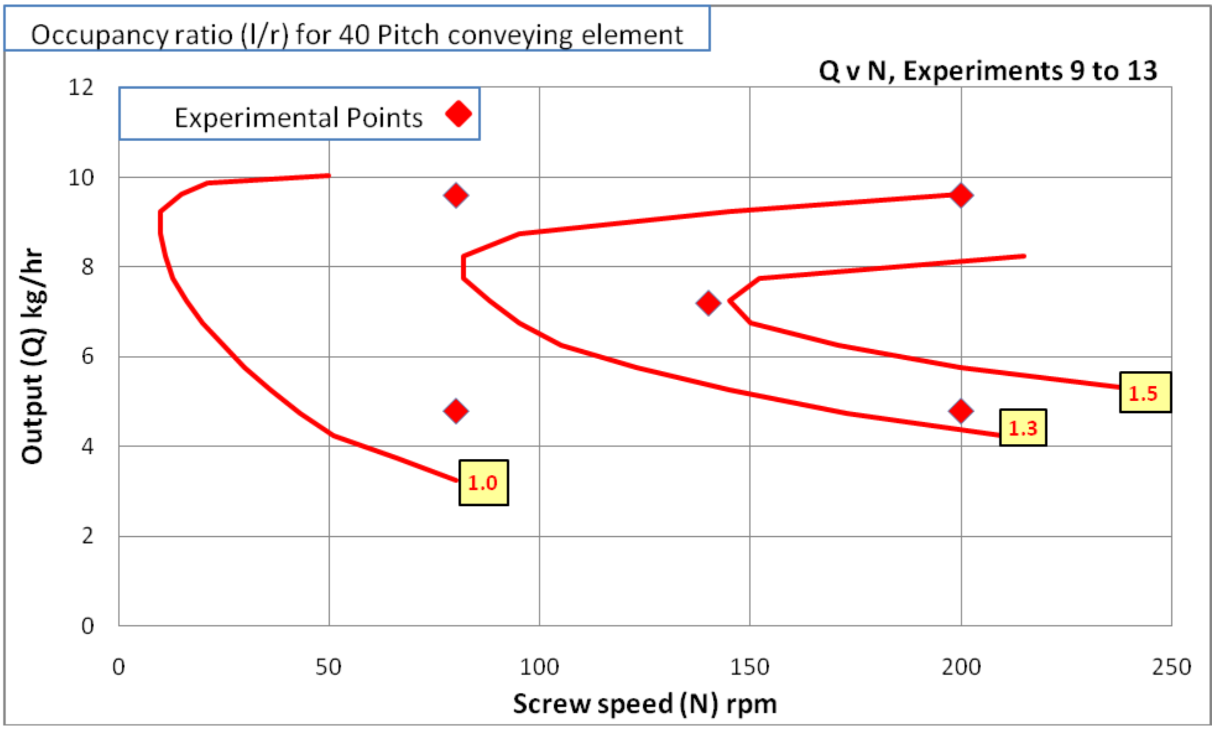


Figure 4-1-11 Occupancy Ratio for 40 pitch conveying element

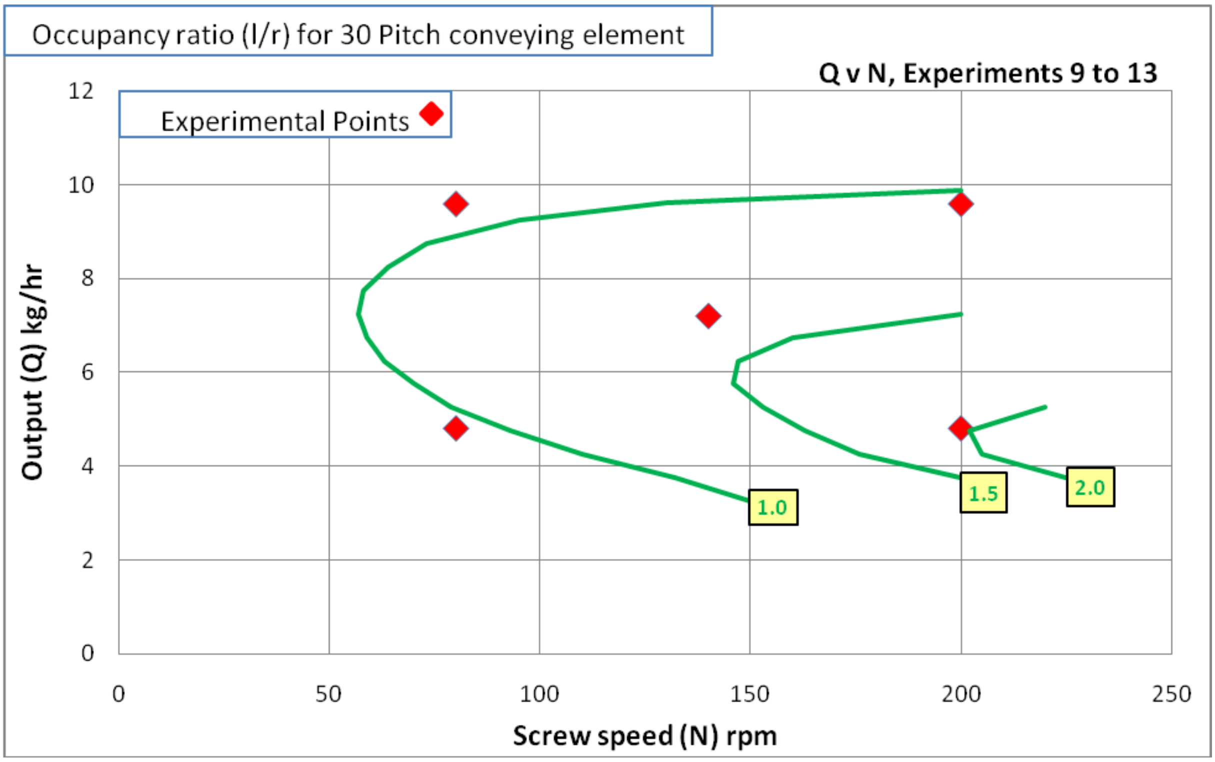


Figure 4-1-12 Occupancy Ratio for 30 pitch conveying element

4.2 Comparing with 1D Simulation results for Kneading Blocks

4.2.1 General processing conditions

The following tables, 4-2-1 and 4-2-2, give an overview of the data extracted from the summary spreadsheet for each experiment 02 to 08. The variables are the same ones that were analysed for the conveying elements in experiments 09 to 13, and will be treated in the same way to enable a comparison to be drawn between the conveying elements and the kneading blocks.

Element Tested	60° forwarding kneading block						
Experiment Number	2	3	4	5	6	7	8
Feed rate (kg/hr)	2.4	4.8	4.8	9.6	4.8	9.6	9.6
Screw speed (rpm)	40	80	120	200	200	80	120
Number of runs	30	50	48	26	24	20	30
Standard error	18.3%	14.1%	14.4%	19.6%	20.4%	22.4%	18.3%
Rt Mean (secs)	10.106	6.200	4.475	2.909	3.620	3.269	3.127
Rt Median (secs)	8.249	4.042	3.706	2.790	3.611	2.858	2.647
Rt Standard deviation	9.278	8.843	2.261	0.798	1.154	1.025	1.354
Coefficient of Variation	0.92	1.43	0.51	0.27	0.32	0.31	0.43
XY/XYZ Mean	0.939	0.938	0.951	0.983	0.979	0.948	0.982
XY/XYZ Std deviation	0.026	0.021	0.021	0.007	0.007	0.025	0.006
XY/XYZ Coef. Of variation	0.028	0.022	0.022	0.007	0.007	0.026	0.006
Average velocity (mm/s)	34.9	67.8	84.3	207.1	177.2	87.4	128.3
Max acceleration (mm^2/s)k	3.7	12.7	4.4	36.4	166.8	43.2	7.1
Occupancy left/right	1.033	0.894	0.996	1.020	1.066	0.835	1.037
Pbs	0.345	0.526	1.080	0.684	1.864	0.706	0.885
Tip passes	1.310	0.263	0.040	2.053	0.727	7.118	2.231
Pbs + Tip passes	1.655	0.789	1.120	2.737	2.591	7.824	3.116
Ratio velocity>threshold	0.80%	1.00%	0.00%	0.10%	0.00%	4.40%	0.00%
% Tip passes	0.1%	0.1%	0.0%	0.4%	0.2%	0.80%	1.10%

Table 4-2-1 Data for 60° forwarding kneading block (experiments 2 to 8)

Element Tested	90° neutral kneading block						
Experiment Number	2	3	4	5	6	7	8
Feed rate (kg/hr)	2.4	4.8	4.8	9.6	4.8	9.6	9.6
Screw speed (rpm)	40	80	120	200	200	80	120
Number of runs	30	50	48	26	24	20	30
Standard error	18.3%	14.1%	14.4%	19.6%	20.4%	22.4%	18.3%
Rt Mean (secs)	10.837	7.790	7.337	3.075	5.581	3.516	3.139
Rt Median (secs)	9.403	4.957	6.060	2.953	4.884	3.491	2.942
Rt Standard deviation	4.392	8.402	5.639	0.796	2.105	1.075	0.884
Coefficient of Variation	0.41	1.08	0.77	0.26	0.38	0.31	0.28
XY/XYZ Mean	0.944	0.941	0.960	0.983	0.975	0.939	0.979
XY/XYZ Std deviation	0.022	0.026	0.020	0.006	0.010	0.039	0.007
XY/XYZ Coef. Of variation	0.023	0.028	0.021	0.006	0.010	0.042	0.007
Average velocity (mm/s)	31.6	60.3	78.9	179.1	137.8	83.1	107.9
Max acceleration (mm^2/s)k	3.8	13.2	4.4	33.8	16.9	45.6	8.0
Occupancy left/right	0.988	1.119	0.912	1.049	0.988	0.977	1.058
Pbs	0.793	0.632	1.000	1.368	2.364	1.353	0.769
Tip passes	1.069	0.368	0.080	0.684	0.000	18.882	0.538
Pbs + Tip passes	1.862	1.000	1.080	2.052	2.364	20.235	1.307
Ratio velocity>threshold	0.60%	0.40%	0.00%	0.10%	0.00%	4.40%	0.00%
% Tip passes	0.10%	0.10%	0.00%	0.10%	0.00%	1.50%	0.20%

Table 4-2-2 Data for 90° neutral kneading block (experiments 2 to 8)

4.2.2 Residence Times

The following illustrations (Figures 4-2-1 to 4-2-8) show the screw profile, as modelled on 'Ludovic' that was used to examine the kneading blocks. They also show plots of melt temperature, and local residence time for each of the seven operating conditions used in experiments 02 to 08.

From these simulations it was possible to obtain the predicted total residence time for the whole screw and to plot contour lines for residence time on the graph of output vs screw speed, (Figure 4-2-9). This is a repeat of the analysis carried out for the conveying elements in experiments 9 to 13, and shown in figure 4-1-7. This figure is reproduced alongside figure 4-2-8 so that a comparison can be made between the two screws, which only differed by the insertion of three kneading blocks in place of three conveying elements.

The pattern is similar, but it can easily be seen that the overall residence time was more for the kneading blocks than for the conveying elements. This is to be expected as the 90° kneading elements ensure that the section under the Pept window is full of polymer, thus increasing the total residence time of the screw.

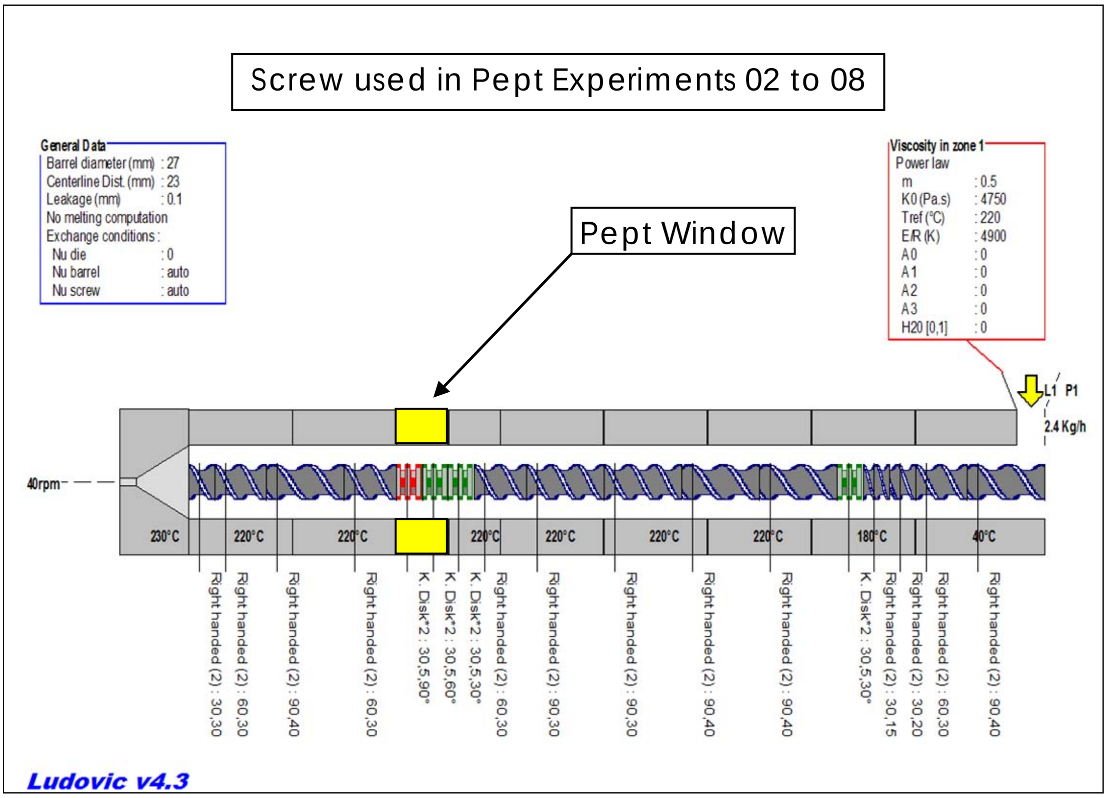


Figure 4-2-1 Screw used in Pept Experiments 2 to 8

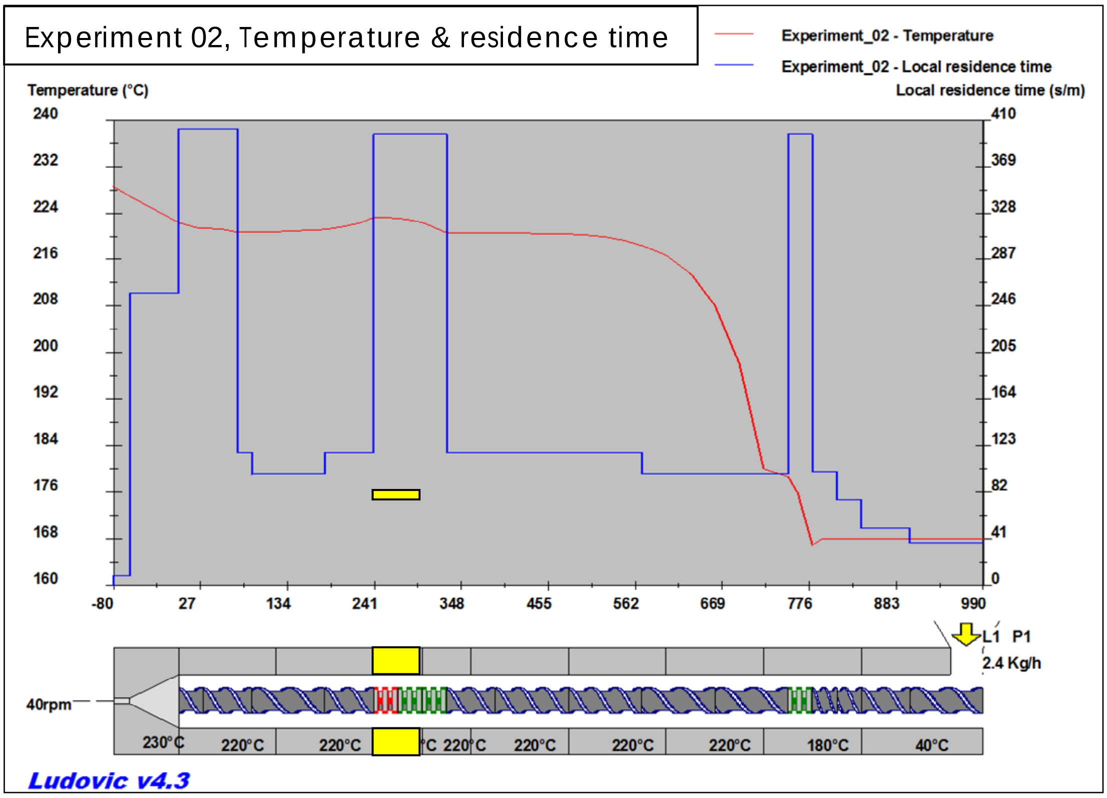


Figure 4-2-2 Ludovic prediction for Experiment 02

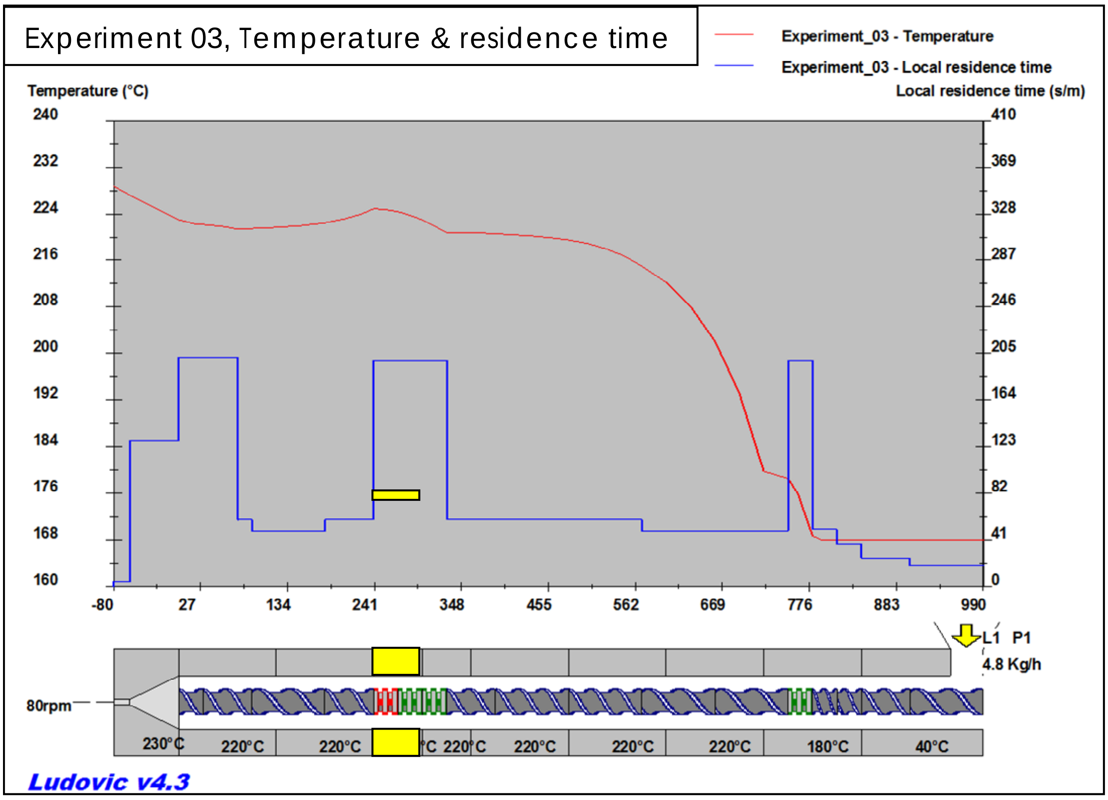


Figure 4-2-3 Ludovic prediction for Experiment 03

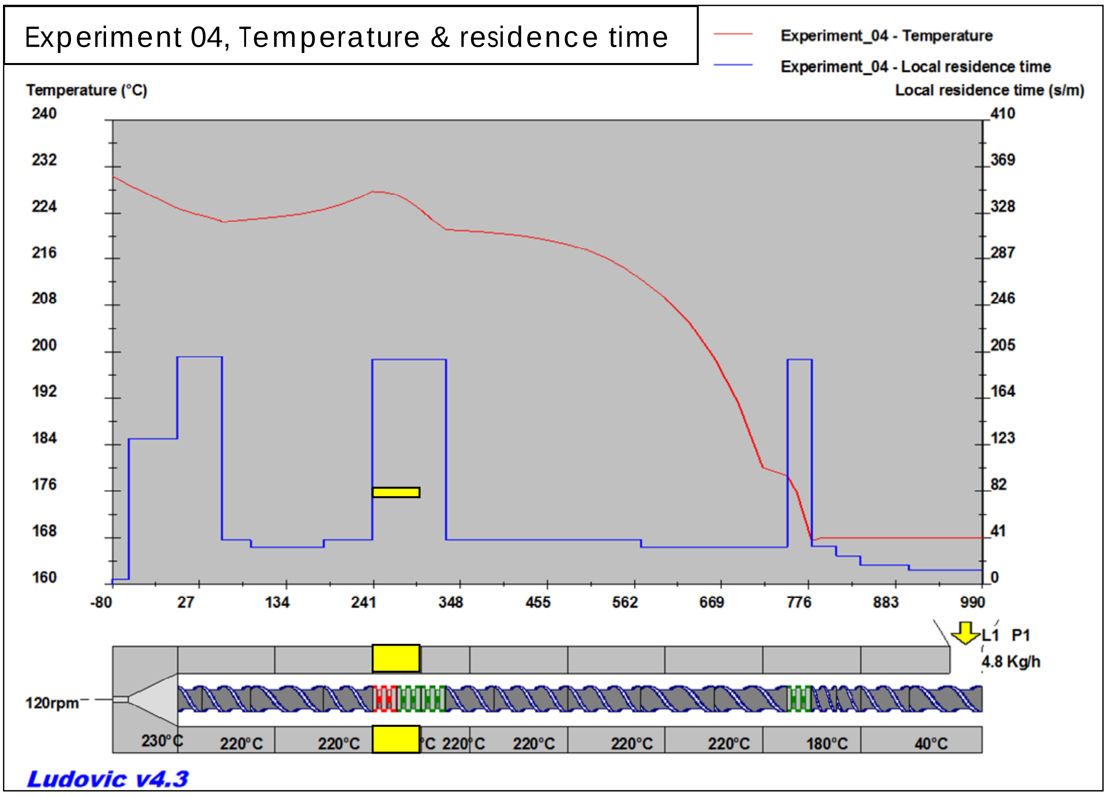


Figure 4-2-4 Ludovic prediction for Experiment 04

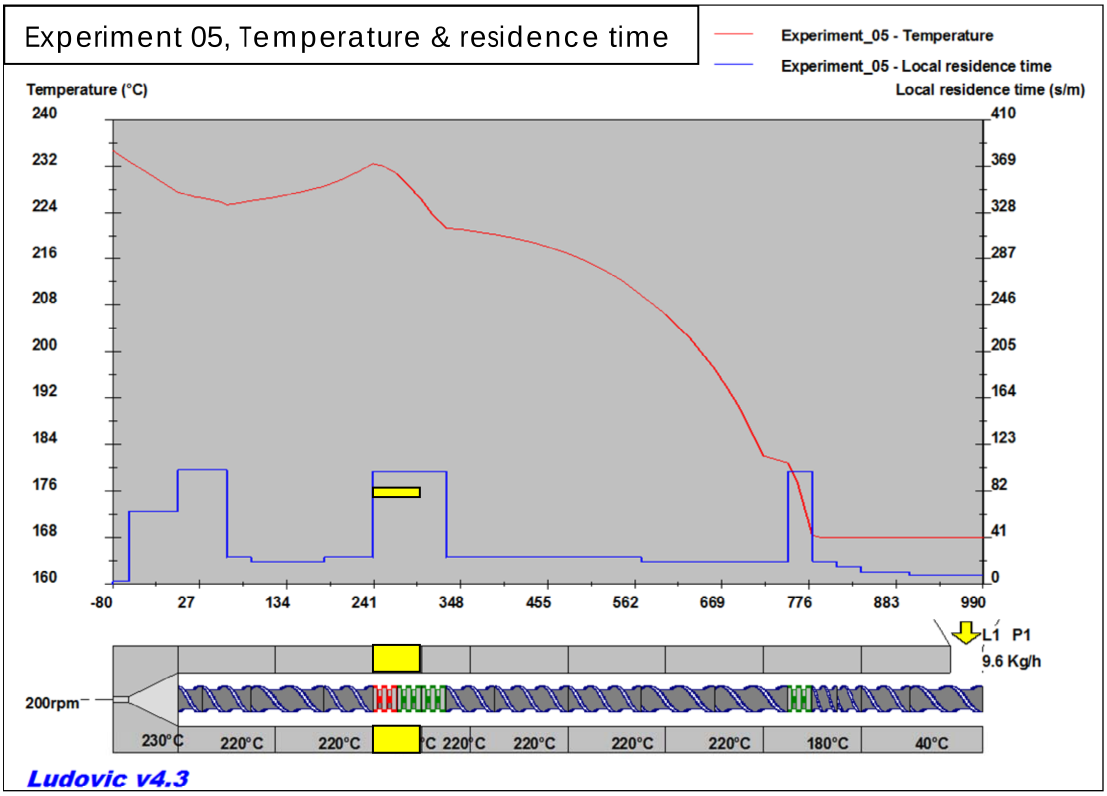


Figure 4-2-5 Ludovic prediction for Experiment 05

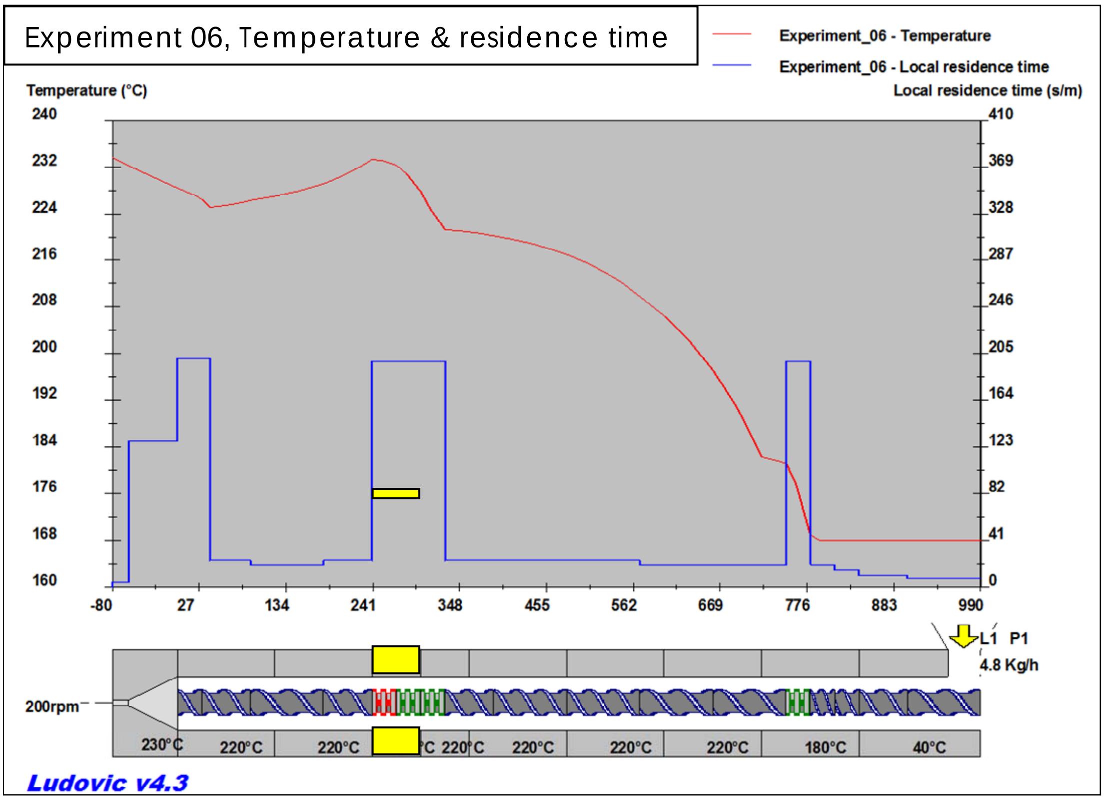


Figure 4-2-6 Ludovic prediction for Experiment 06

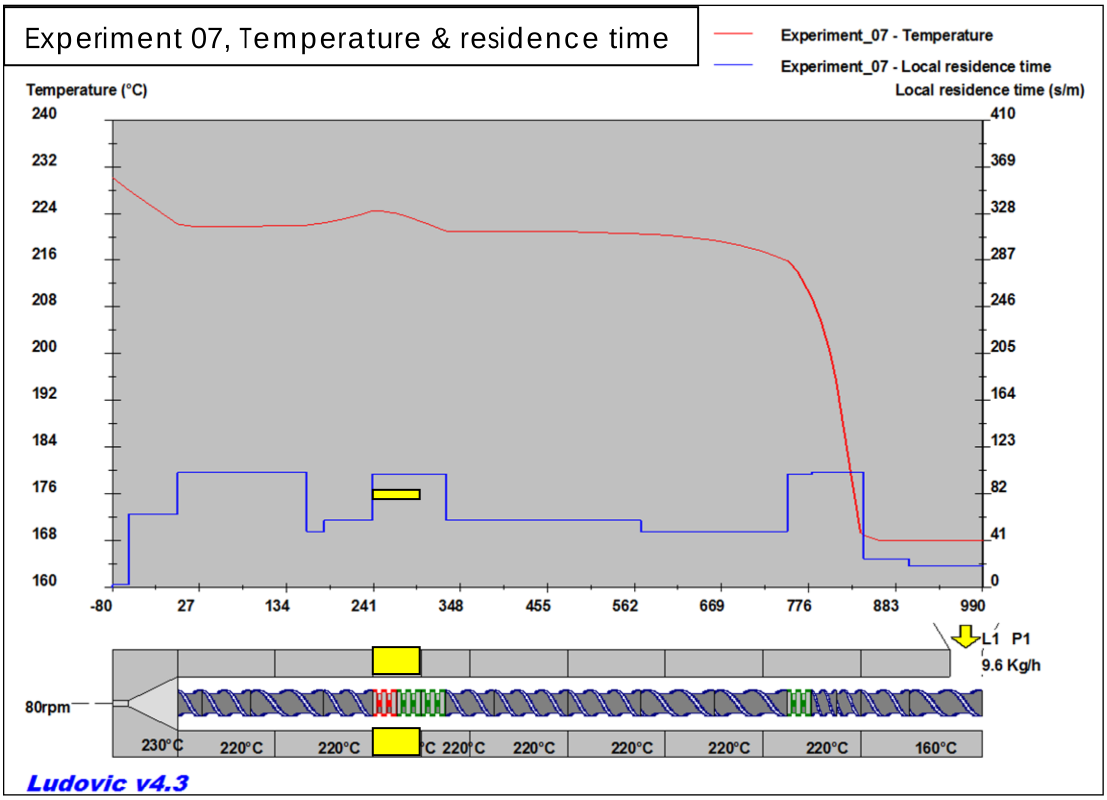


Figure 4-2-7 Ludovic prediction for Experiment 07

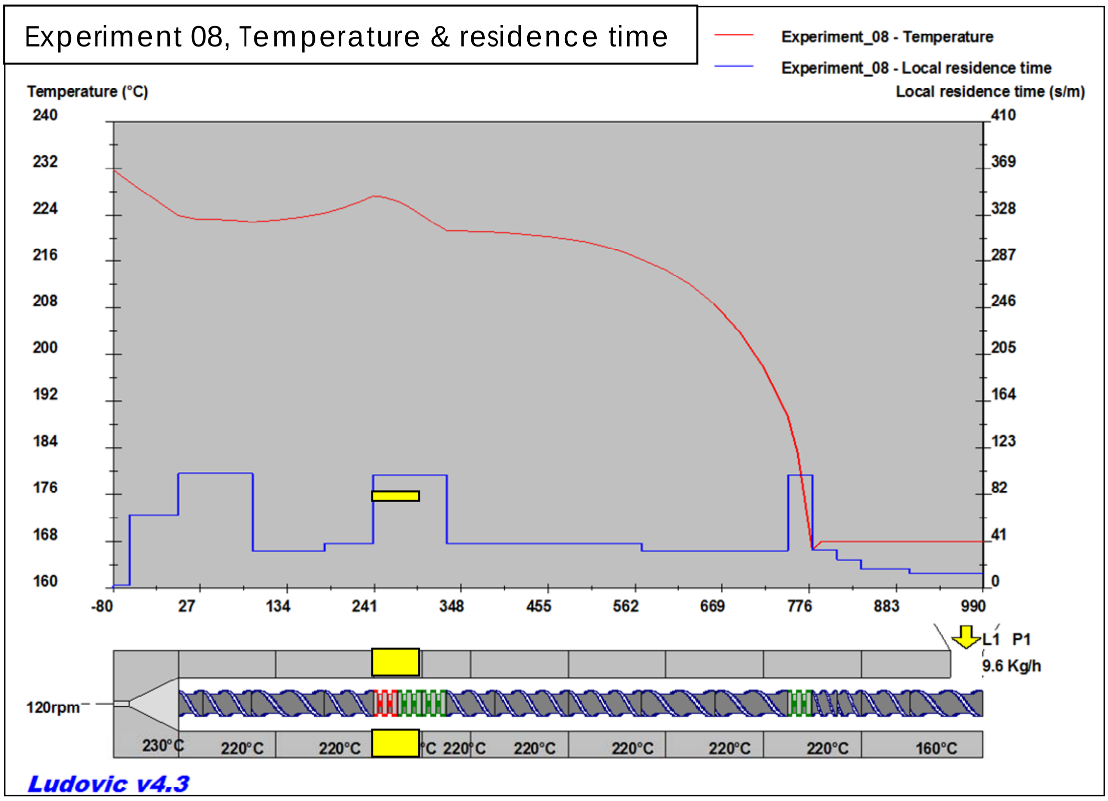


Figure 4-2-8 Ludovic prediction for Experiment 08

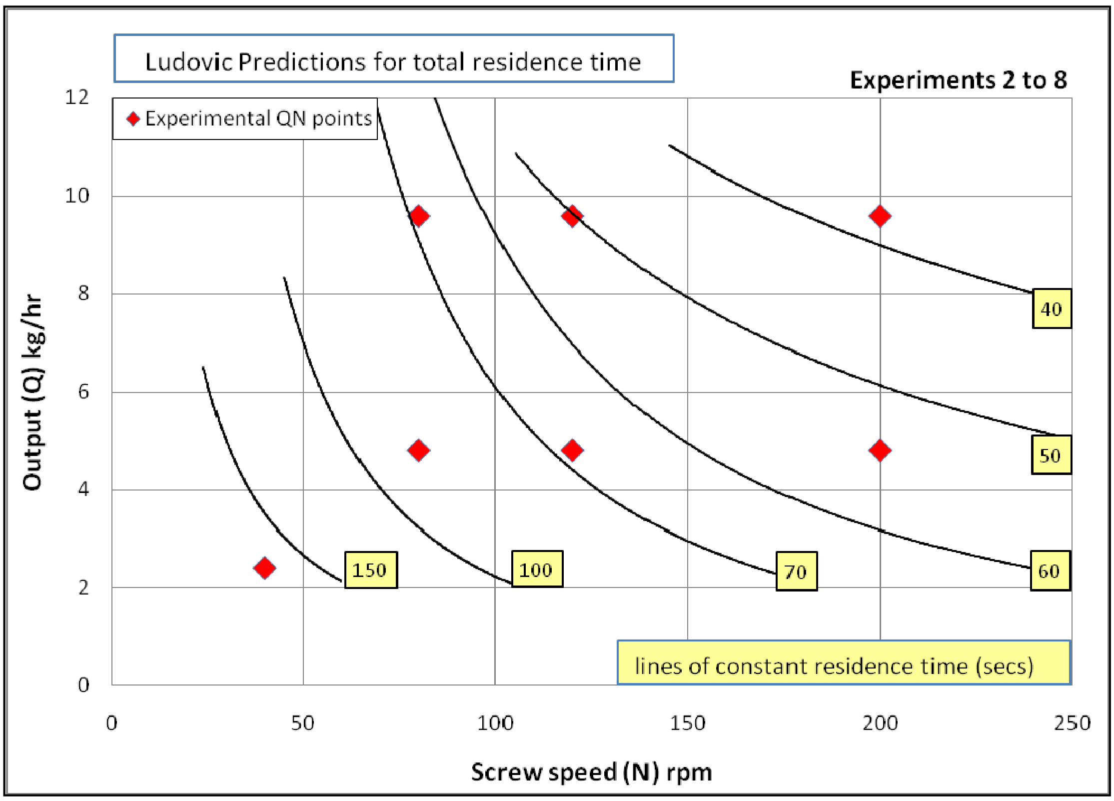


Figure 4-2-9 Ludovic prediction for total residence time (2 to 8) - Kneading Blocks

Figure 4-2-10 Ludovic prediction for total residence time (9 to 13) - Conveying elements (Repeat of figure 4-1-7)

As mentioned, in the earlier section dealing with the conveying elements and experiments 9 to 13, the Pept experiments were only able to measure the residence times under the Pept window. Therefore the same treatment was given to the kneading block experiments, and graphs of residence times, for the 60° forwarding block and the 90° neutral block, were prepared. These include both the 'Ludovic' predictions and the actual Pept measurements. (Figures 4-2-11 and 4-2-12)

Again, as for the conveying elements, there are areas where the 'Ludovic' predictions and the Pept measurements have close agreement. However, they drift apart at the lower screw speeds and throughputs. Bearing in mind that the 'Ludovic' software is essentially 'one dimensional', to enable fast simulations to be conducted with minimum computing power, then the agreement with Pept measurements is very good.

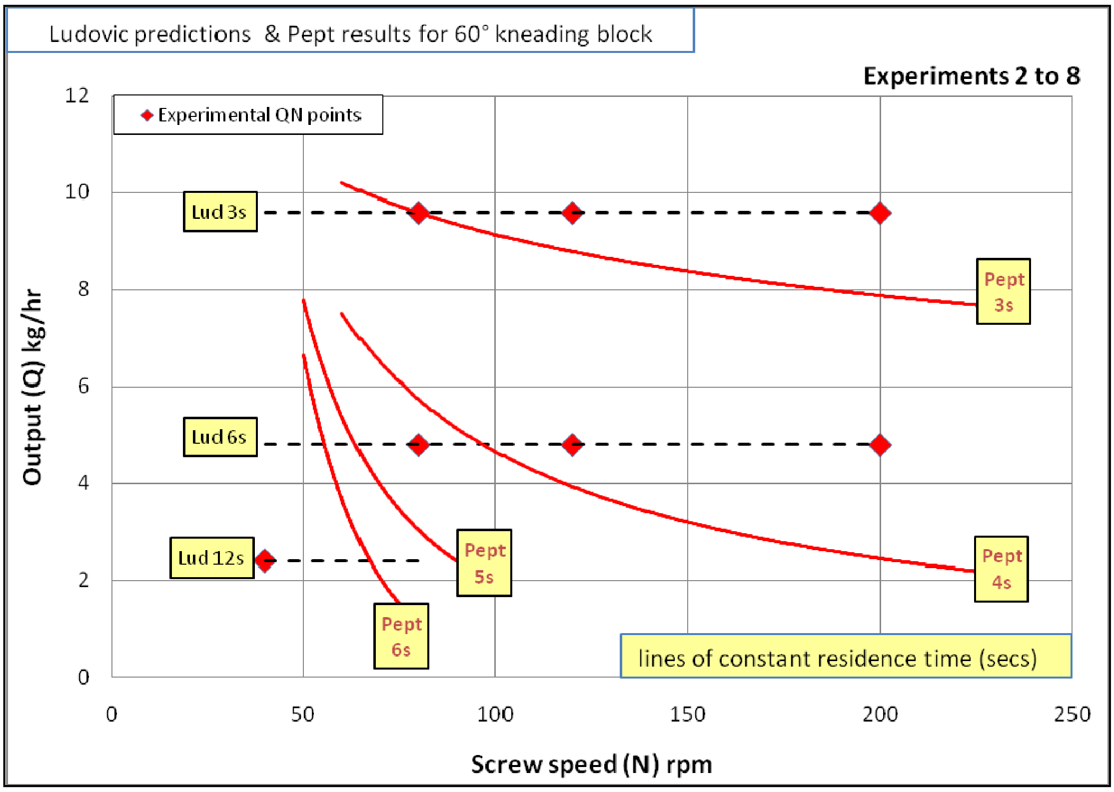


Figure 4-2-11 Residence times for 60° forwarding kneading block

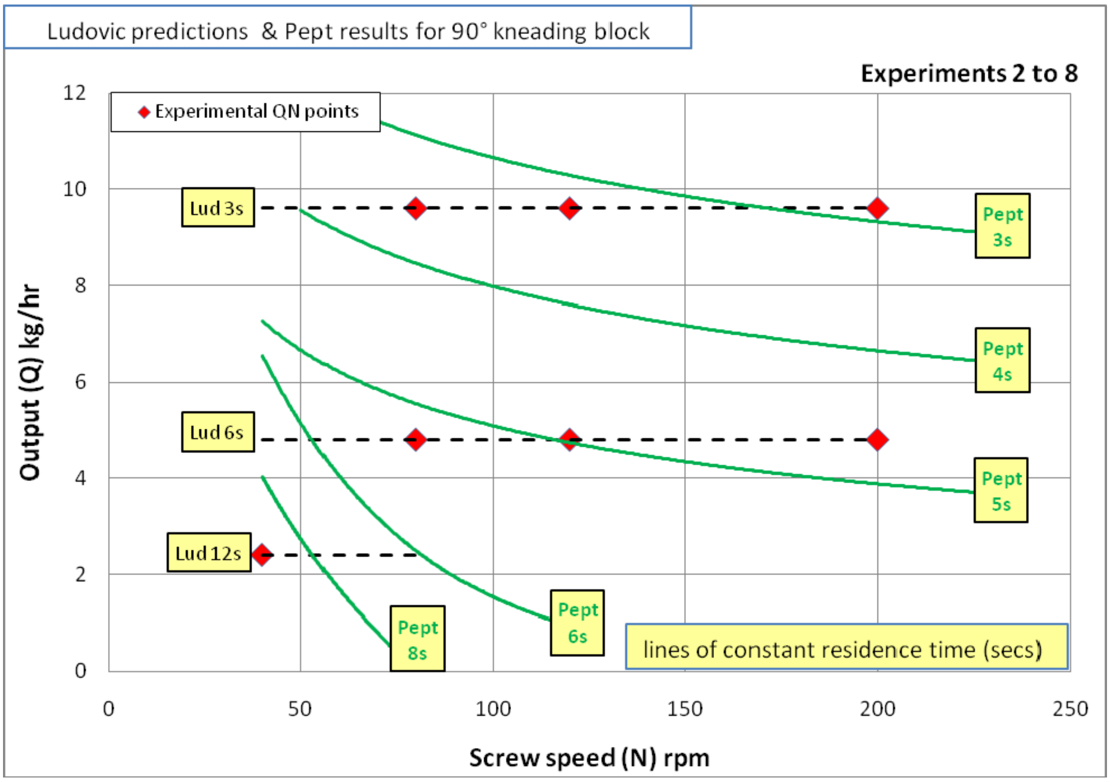


Figure 4-2-12 Residence times for 90° neutral kneading block

4.2.3 Occupancy Ratio

By monitoring the position of the particle, and recording which quadrant of the twin screw it was in at any one time, it was possible to measure how long the particle resided in the left hand screw and how long in the right when viewed from the discharge end of the extruder. The ratio, of left hand screw over right hand screw, is included in the table of data for the 60°, and the 90° kneading blocks. Tables 4-2-1 and 4-2-2.

Upon examination it is clear that they are all around 1.0 thus implying that there was equal occupancy on both screws. This was not surprising as the 90° block is a neutral block with no conveying ability, hence it would be full and reliant upon downstream elements to push the polymer through. Equally the 60° block has only a limited conveying capacity and would not have enough to overcome the resistance of the 90° block, hence it would also be full. Thus if both elements are full then both screws must also be full in that region, therefore we would expect the occupancy ratio of left/right to equal one.

Based on this, it is possible that we could use this ratio to decide when an element is full. If the number is consistently greater than one then this would indicate that the screws were not full. Also with the ratio always close to one then there is a high probability that the screws are full.

Finally we can use the standard error to show that the variation seen, between all seven conditions examined, is not significant and that the ratio is nominally equal to one. The standard error, calculated from the number of runs, varies from a minimum of 14% to a maximum of 22%, say an average of 18%. By plotting the results and imposing lines of ± 18% it can readily be seen that all the results lie within these two limits thus showing that the differences are not significant. (Figure 4-2-13)

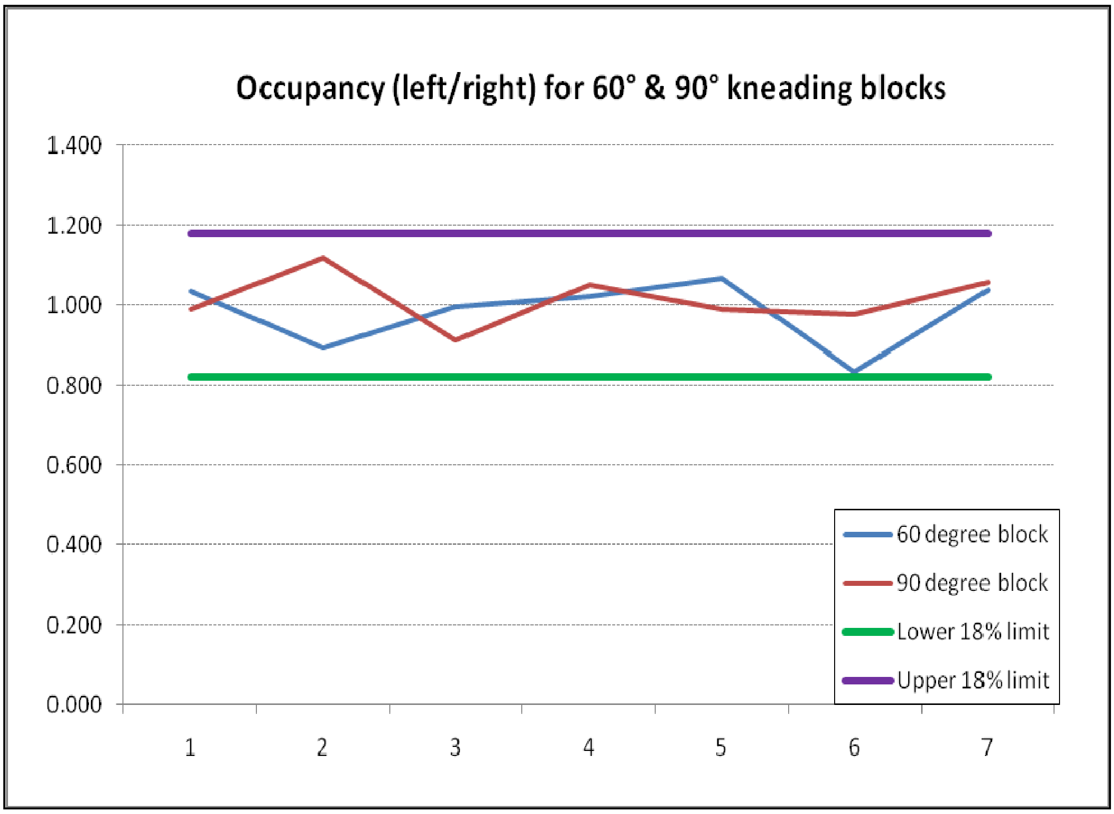


Figure 4-2-13 Occupancy of 60° and 90° kneading blocks, when full.

4.2.4 Conclusion and Outlook

Twin Screw simulation is often regarded as not very applicable for practical use, due to numerous reasons:

- Material data difficult to determine
- Material data varying to much along the flow path
- Results affected by processes that are impossible to model (Melting, Mixing two medias, etc.)
- Results sometimes completely unrealistic even for important processing characteristics (e.g. melt temperature)
- 1D Simulation Systems such as Ludovic seem to predict the residence time in the observed section with high accuracy

5 An approach to calculate mixing efficiency from PEPTFlow results

5.1 From PEPTFlow results to Mixing efficiency for Conveying elements

There are a variety of indicators that have been included as possible measures of mixing, both distributive and dispersive. Some of these are already accepted within the compounding industry, and others have been suggested in discussion between members of the consortium.

None of the assumptions made, when arriving at these mixing numbers, have yet been proven by PeptFlow, so what follows is essentially a theory for evaluating the screw designs ability to deliver dispersive and distributive mixing, that will be examined further by some of the case studies.

Details about how these numbers were evaluated can be found in the following sections on Distributive and Dispersive mixing. Tables were constructed for each of the two conveying elements examined in experiments 9 to 13, and graphs then prepared to show how these mixing numbers were affected by changes in running conditions.

Element Tested	40pr				
Experiment Number	9	10	11	12	13
Feed rate (kg/hr)	4.8	4.8	9.6	9.6	7.2
Screw speed (rpm)	80	200	200	80	140
Rt Coef. of Variation	0.51	1.32	0.52	0.85	0.56
XY/XYZ Coef. of variation	0.04	0.54	0.18	0.04	0.03
Distributive Mixing Total	**0.550**	**1.865**	**0.697**	**0.889**	**0.591**
Average velocity (mm/s)	87.9	139.9	197.8	87.0	138.2
Score out of 20	8.8	14.0	19.8	8.7	13.8
Max acceleration (mm^2/s)k	148.49	11.80	70.56	72.40	89.35
Score out of 20	29.70	2.36	14.11	14.48	17.87
% Tip passes	0.30%	0.00%	0.30%	0.50%	0.40%
Score out of 10	3	0	3	5	4
Dispersive Mixing Total	**41.4879**	**16.3500**	**36.8912**	**28.1820**	**35.6915**

Table 5-1-1, Mixing Numbers for 40 pitch conveying element.

Element Tested	30pr				
Experiment Number	9	10	11	12	13
Feed rate (kg/hr)	4.8	4.8	9.6	9.6	7.2
Screw speed (rpm)	80	200	200	80	140
Rt Coef. of Variation	0.81	0.60	0.61	0.37	0.55
XY/XYZ Coef. of variation	0.05	0.35	0.19	0.04	0.03
Distributive Mixing Total	**0.861**	**0.949**	**0.807**	**0.404**	**0.586**
Average velocity (mm/s)	84.8	152.3	176.6	84.1	132.3
Score out of 20	8.5	15.2	17.7	8.4	13.2
Max acceleration (mm^2/s)k	98.47	15.20	66.91	66.73	82.72
Score out of 20	19.69	3.04	13.38	13.35	16.54
% Tip passes	0.90%	0.20%	0.70%	0.90%	0.20%
Score out of 10	9	2	7	9	2
Dispersive Mixing Total	**37.1786**	**20.2685**	**38.0387**	**30.7613**	**31.7774**

Table 5-1-2, Mixing Numbers for 30 pitch conveying element.

5.1.1 Distributive Mixing

Firstly distributive mixing which, as its name implies, is a measure of how well the various ingredients are distributed throughout the matrix. The first indicator of distributive mixing is the coefficient of variation of the residence time. This is a dimensionless version of the residence time standard deviation, and effectively gives a measure of the ‘end to end’ mixing that has taken place. Also included is the ratio, (XY/XYZ) which gives an indication of how far the particle travels across the cross-section of the screw in relation to the total distance travelled whilst traversing that element. Again the coefficient of variance is used to enable a dimensionless version to be used of this measure of (side to side?) mixing. In order to obtain a number, which could be plotted against various factors, these two coefficients were added together to give a ‘distributive mixing number’. This was then plotted against throughput and screw speed in figures 60 and 61.

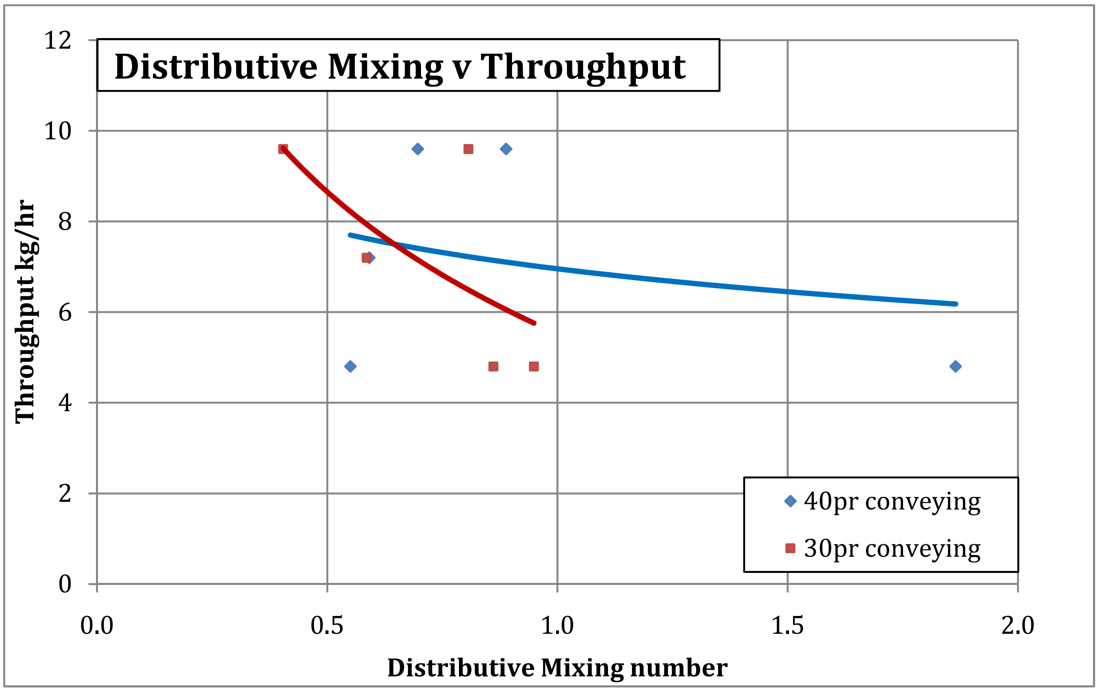


Figure 5-1-1 Distributive Mixing v Throughput

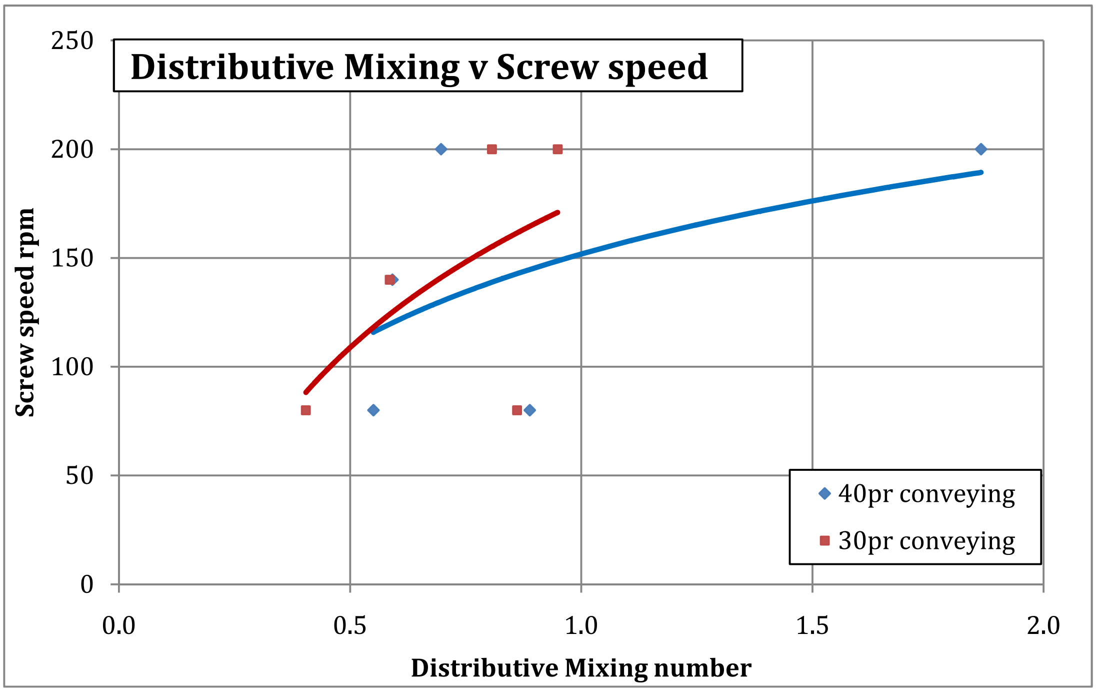


Figure 5-1-2 Distributive Mixing v Screw Speed

It is difficult to draw firm conclusions as there is a lot of scatter, however the trend lines do point to some tentative trends that will need to be examined in the future. These are that Distributive mixing appears to increase with decreasing throughput and increasing speed. Hence, the best distribution would be obtained, with conveying elements, at high speed and low throughput. This condition is found in experiment 10 which does show the highest distribution number.

5.1.2 Dispersive Mixing

Secondly dispersive mixing, which is more to do with breaking up agglomerates, and spreading particles within the matrix. This type of mixing requires high shear rates for short periods of time, or stretching flows, typified by high acceleration of the particle. The three main indicators used are average velocity, to give a view on relative shear rates, maximum acceleration, as a measure of stretching flow, and %tip passes, which incorporate high shear and stretching flow. Unfortunately errors are possible with two of these indicators. The maximum acceleration has cumulative error, as it is a measure of a small difference in two velocities, which are themselves subject to errors in the short difference between two times. Also the tip passes are dependent upon the particle having a velocity greater than the tip velocity, (See Appendix 1) as well as being in a position outside of the diameter of the screw flight. Hence more cumulative error is possible.

To establish a 'Dispersive mixing number' that could be used as a comparator with other elements it was necessary to assign an arbitrary figure to the three different indicators and then use the sum of the assigned numbers. Looking at the variations in the three key indicators, and making a judgement on the relative importance of the indicators chose the following figures chosen;

1. Tip passes of 1% score 10 reducing to a score of zero for 0% tip passes.
2. Max. Acceleration of 50,000 mm2/sec scores 10, with pro rata reduction down to zero for zero acceleration.
3. Avg. Velocity of 100 mm/sec scores 10, again with pro rata reduction to zero for zero velocity.

These numbers were then added together to give a 'Dispersive mixing number', which was then plotted against throughput (Figure 62) and screw speed (Figure 63). It should be stressed that this number has only been used in order to enable comparisons to be made, both here, and later when examining kneading blocks and different elements. It is not a number that is in common use anywhere, and will need to be adjusted in response to the results from further practical experiments.

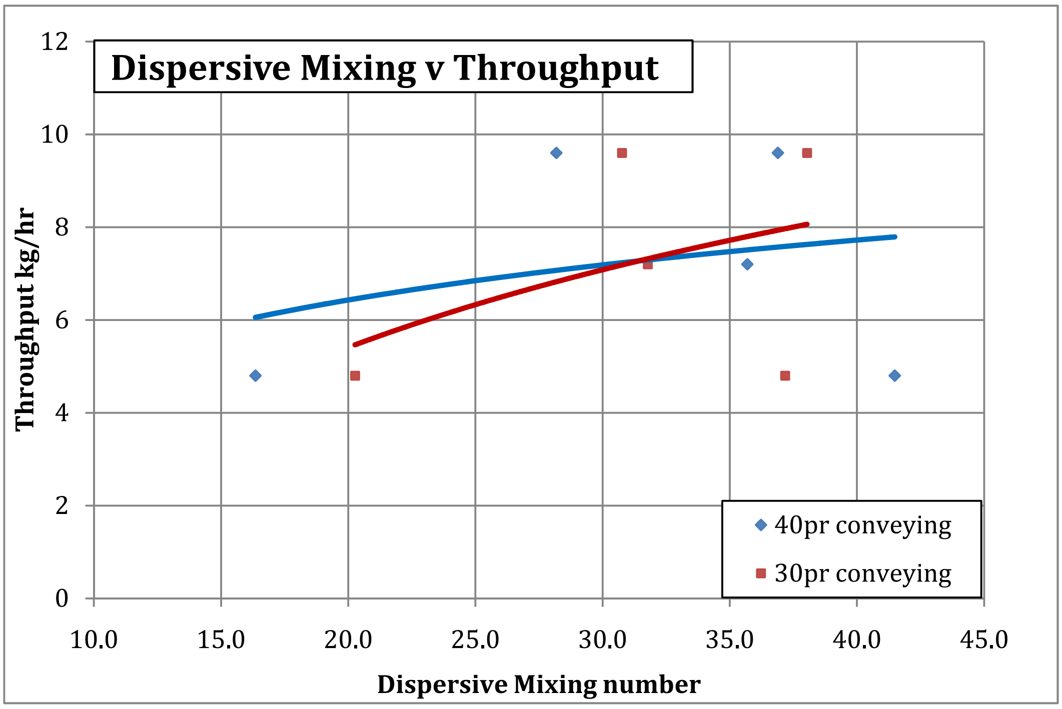


Figure 5-1-3 Dispersive Mixing v Throughput

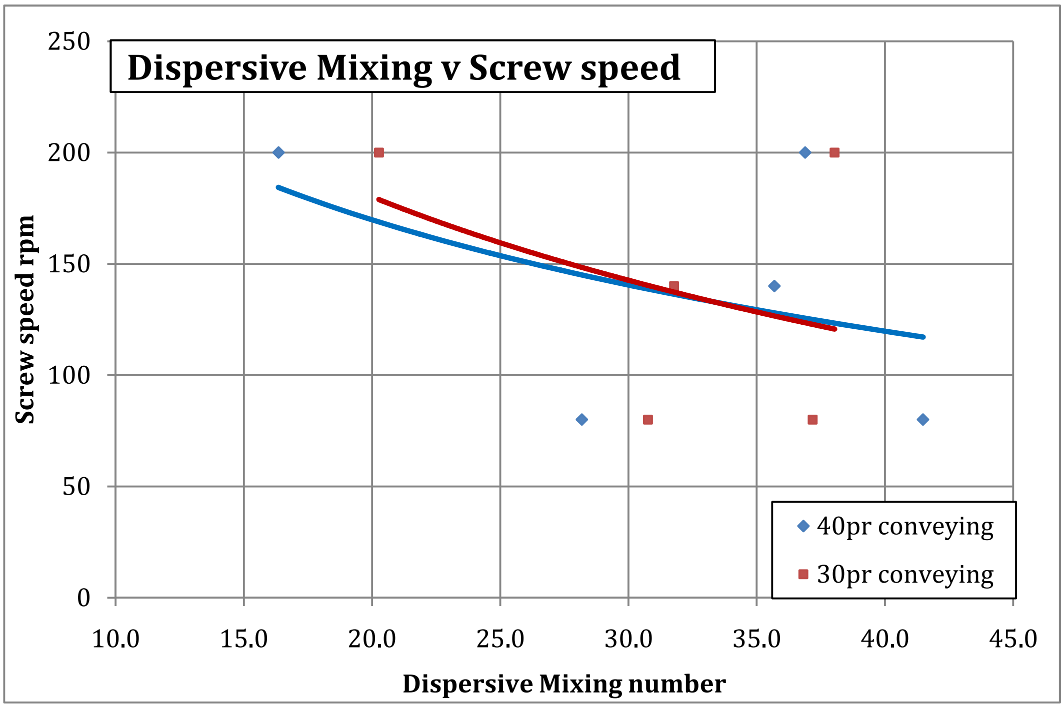


Figure 5-1-4 Dispersive Mixing v Screw Speed

As for distributive mixing, it is difficult to draw firm conclusions, as there is a lot of scatter, however the trend lines do point to some tentative trends that will need to be examined in the future. These are that the Dispersive mixing appears to increase with increasing throughput and decreasing speed. Hence the best dispersion would be obtained, with conveying elements, at low speed and high throughput.

The general conclusion, that high speed and low throughput gives greater distributive mixing but lower dispersive mixing, when running a predominantly conveying element screw, is already understood within the industry. Essentially these conditions allow for a partly full screw where the end-to-end mixing of the conveying elements is given room to operate and therefore produce good distribution. On the other hand the partly empty screws mean that there is less material passing over the tips, and fewer high-pressure areas where acceleration can produce stretching flows. Hence there is less dispersive mixing.

5.2 From PEPTFlow results to Mixing efficiency for Kneading discs

There are a variety of indicators that have been included as possible measures of mixing, both distributive and dispersive. As discussed earlier, in the section on conveying elements, none of these indicators have yet been proven by PeptFlow, so what follows is essentially a theory for dispersive and distributive mixing that will be examined further by some of the case studies.

In the same way, as for the conveying elements, tables were constructed for each of the two sets of kneading blocks tested in experiments 2 to 8, and graphs then prepared to show how these mixing numbers were affected by changes in running conditions. The calculated mixing numbers are shown in the following two tables 5-2-1 & 5-2-2.

Element Tested	60° forwarding kneading block						
Experiment Number	2	3	4	5	6	7	8
Coeff of variation Rt	0.918	1.426	0.505	0.274	0.319	0.314	0.433
Coeff of variation XY/XYZ	0.028	0.022	0.022	0.007	0.007	0.026	0.006
Distributive Mixing Total	**0.946**	**1.449**	**0.527**	**0.281**	**0.326**	**0.340**	**0.439**
Average velocity (mm/s)	34.9	67.8	84.3	207.1	177.2	87.4	128.3
Score out of 20	3.5	6.8	8.4	20.7	17.7	8.7	12.8
Max acceleration (mm^2/s)k	1.4	5.4	4.1	23.9	17.3	50.5	4.5
Score out of 20	0.3	1.1	0.8	4.8	3.5	10.1	0.9
% Tip passes	0.1%	0.1%	0.0%	0.4%	0.2%	0.8%	1.1%
Score out of 10	1	1	0	4	2	8	11
Dispersive Mixing Total	**4.8**	**8.9**	**9.3**	**29.5**	**23.2**	**26.8**	**24.7**
Q	2.4	4.8	4.8	9.6	4.8	9.6	9.6
N	40	80	120	200	200	80	120

Table 5-2-1 Mixing Numbers for 60° kneading block (experiments 2 to 8)

Element Tested	90° neutral kneading block						
Experiment Number	2	3	4	5	6	7	8
Coeff of variation Rt	0.405	1.079	0.769	0.259	0.377	0.306	0.282
Coeff of variation XY/XYZ	0.023	0.028	0.021	0.006	0.010	0.042	0.007
Distributive Mixing Total	**0.429**	**1.106**	**0.789**	**0.265**	**0.387**	**0.347**	**0.289**
Average velocity (mm/s)	31.6	60.3	78.9	179.1	137.8	83.1	107.9
Score out of 20	3.2	6.0	7.9	17.9	13.8	8.3	10.8
Max acceleration (mm^2/s)k	1.3	6.7	3.8	20.3	18.4	54.8	4.6
Score out of 20	0.3	1.3	0.8	4.1	3.7	11.0	0.9
% Tip passes	0.1%	0.1%	0.0%	0.1%	0.0%	1.5%	0.2%
Score out of 10	1	1	0	1	0	15	2
Dispersive Mixing Total	**4.4**	**8.4**	**8.7**	**23.0**	**17.5**	**34.3**	**13.7**
Q	2.4	4.8	4.8	9.6	4.8	9.6	9.6
N	40	80	120	200	200	80	120

Table 5-2-2 Mixing Numbers for 90° kneading block (experiments 2 to 8)

5.2.1 Distributive Mixing

Firstly distributive mixing which, as its name implies, is a measure of how well the various ingredients are distributed throughout the matrix. The first indicator of distributive mixing is the coefficient of variation of the residence time. This is a dimensionless version of the residence time standard deviation, and effectively gives a measure of the ‘end to end’ mixing that has taken place. Also the ratio, XY/XYZ, gives an indication of how far the particle travels across the cross-section of the screw in relation to the total distance travelled whilst traversing that element. Again the coefficient of variance is used to enable a dimensionless version to be used of this measure of side-to-side mixing. These two coefficients are added together to give a ‘distributive mixing number’, which is then plotted against throughput and screw speed in figures 5-2-1 and 5-2-2. The data has a large scatter but there is a strong trend towards better distributive mixing at lower throughputs and lower screw speeds. This is different to the trend observed with the conveying elements where lower throughput and **higher speed** gave better distribution.

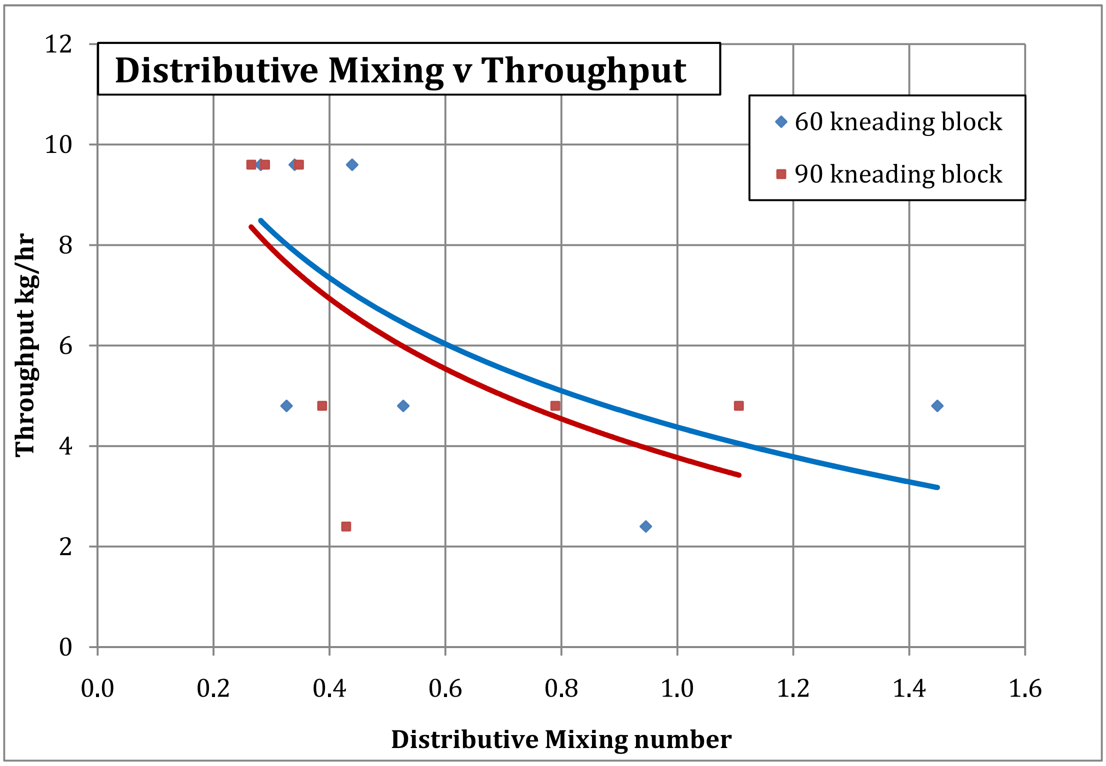


Figure 5-2-1 Distributive mixing v Throughput, with kneading blocks.

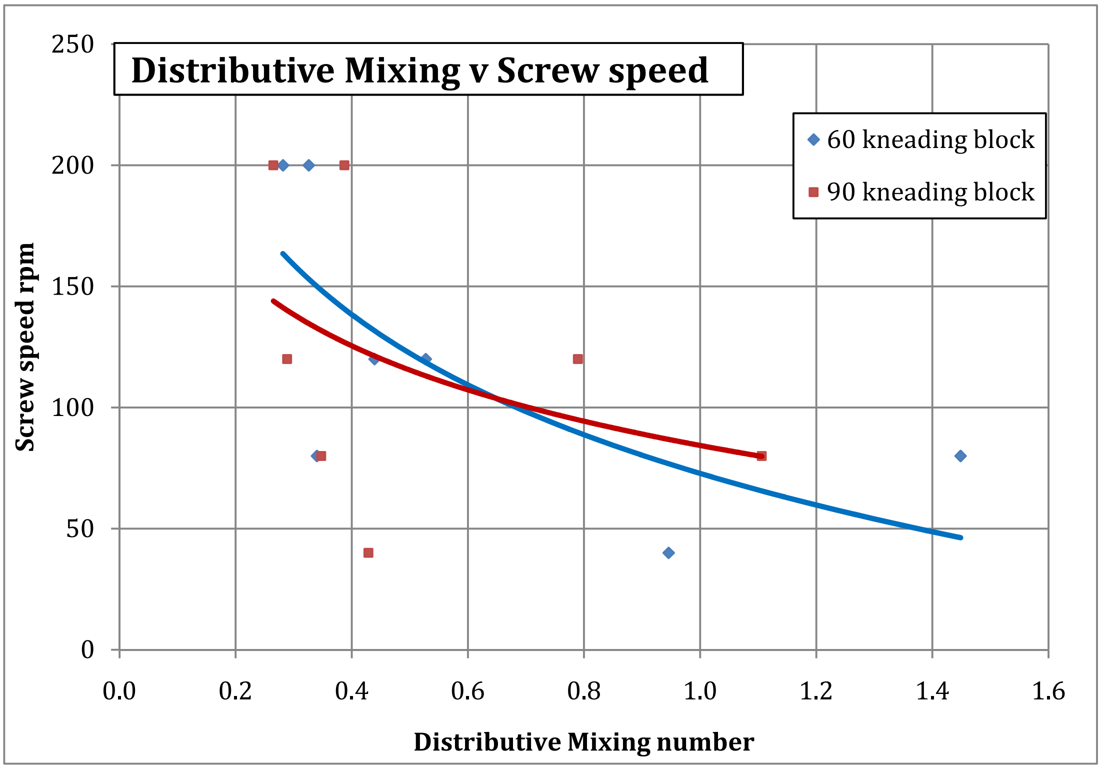


Figure 5-2-2 Distributive mixing v Screw speed, with kneading blocks.

5.2.2 Dispersive Mixing

Secondly dispersive mixing, which is more to do with breaking up agglomerates, and spreading particles within the matrix. This type of mixing requires high shear rates for short periods of time, or stretching flows, typified by high acceleration of the particle. The three main indicators used are average velocity, to give a view on relative shear rates, maximum acceleration, as a measure of stretching flow, and %tip passes, which incorporate high shear and stretching flow. Unfortunately errors are possible with two of these indicators. The maximum acceleration has cumulative error, as it is a measure of a small difference in two velocities, which are themselves subject to errors in the small difference between two times. Also the tip passes are dependent upon the particle having a velocity greater than the tip velocity, as well as being in a position outside of the diameter of the screw flight. Hence more cumulative error is possible.

As for the section on conveying elements, a 'Dispersive mixing number' was calculated using the same criteria and graphs were then plotted for Dispersive mixing against throughput and against screw speed. (Figures 5-2-3 & 5-2-4)

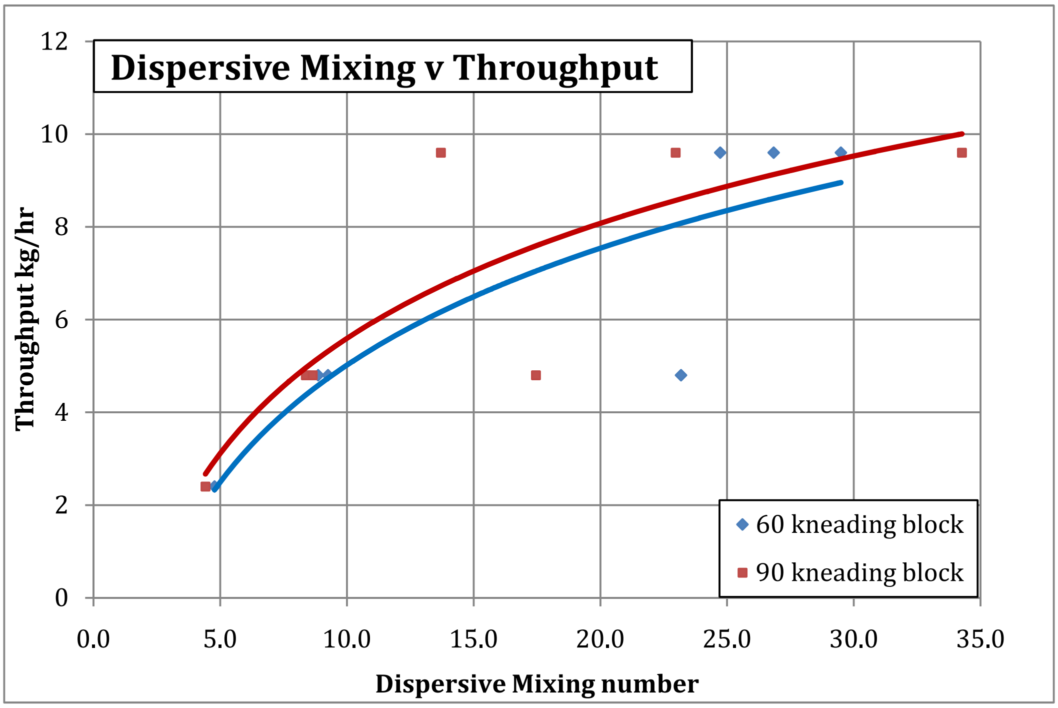


Figure 5-2-3 Dispersive mixing v Throughput, with kneading blocks

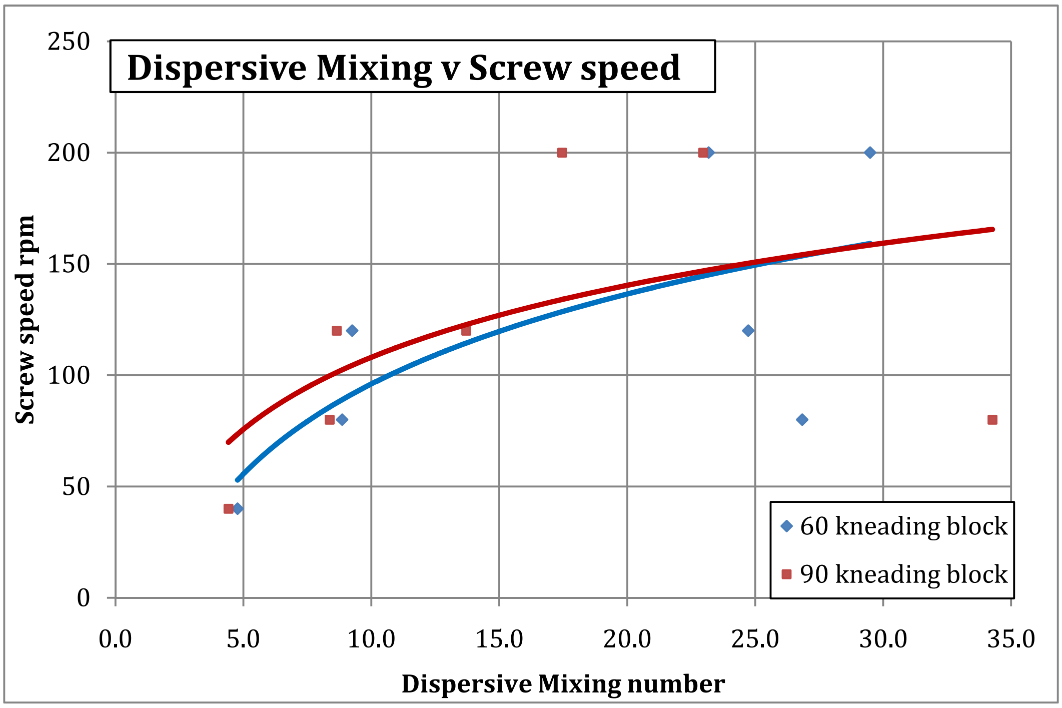


Figure 5-3-4 Dispersive mixing v Screw speed, with kneading blocks

As can be seen from these two figures, dispersive mixing improves with increasing throughput and also with increasing screw speed, which is the opposite with that observed for distributive mixing in figures 5-2-1 and 5-2-2. Essentially, at high speed and high throughput, the screw is often running full, at high shear rates, and with the opportunity for many tip passages, thus giving good dispersion. However, running full will give less end-to-end mixing and hence less distributive mixing. It should be stressed that there is a lot of scatter of both sets of results but the general conclusions do conform to views held already within the compounding industry.

6 Flow phenomena

The following paragraph briefly summarises certain observed flow conditions that show interesting or unexpected flow phenomena. As some of them can have a strong influence on residence time it is important to know that these conditions and phenomena, like those presented, can happen.

6.1 Sticking to the screw

During experiments with the following screw setup

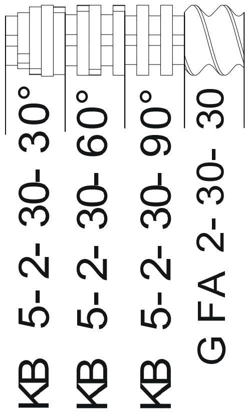


Figure 6-1-1: Screw setup for experiment 3

and the following processing conditions, using the standard PP material a flow path was observed, where the particle was rotating for several revolutions on one screw.

	Experiment 3
Temperature, °C	220-240
Screw speed, 1/min	80
Feedrate, kg/h	4.8

As illustrated in figure 6-1-2 the particle was rotating for 6 revolutions on the left screw.

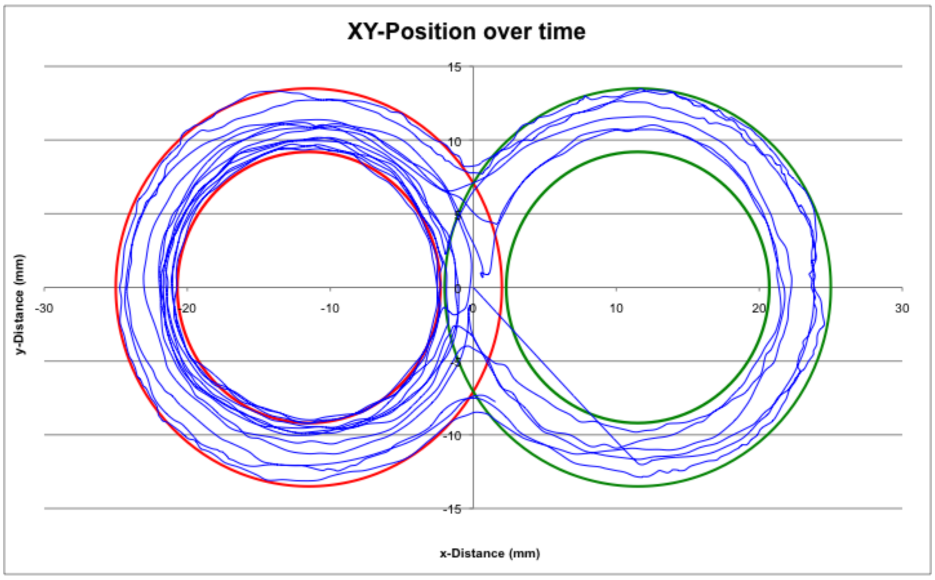


Figure 6-1-2 Particle sticking to the left screw

This condition has led to a passage time that is almost twice as long as the average passage time for this element.

Looking on the following figure 6-1-3 it is quite obvious that the particle got stuck at around 22 seconds and was rotating for more then 13 seconds on one screw. During that time it was only travelling very slowly along the screw, with almost no axial movement between 27 and 33 seconds.

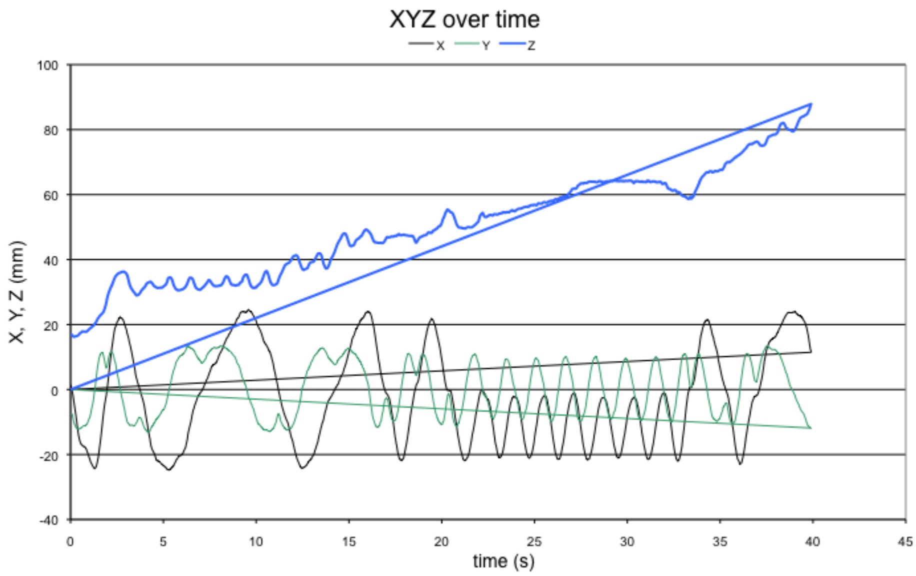


Figure 6-1-3: XYZ-coordinates of a particle stuck on one screw.

Such a flow condition can be a problem with very temperature sensitive material or in reactive processing, where narrow residence time distributions are needed.

6.2 Sticking to the barrel

During the same experiments the following different flow phenomena was observed.

As illustrated in figure 6-1-4 it was slowly but constantly travelling along the eight shape of inner barrel geometry for more than two revolutions.

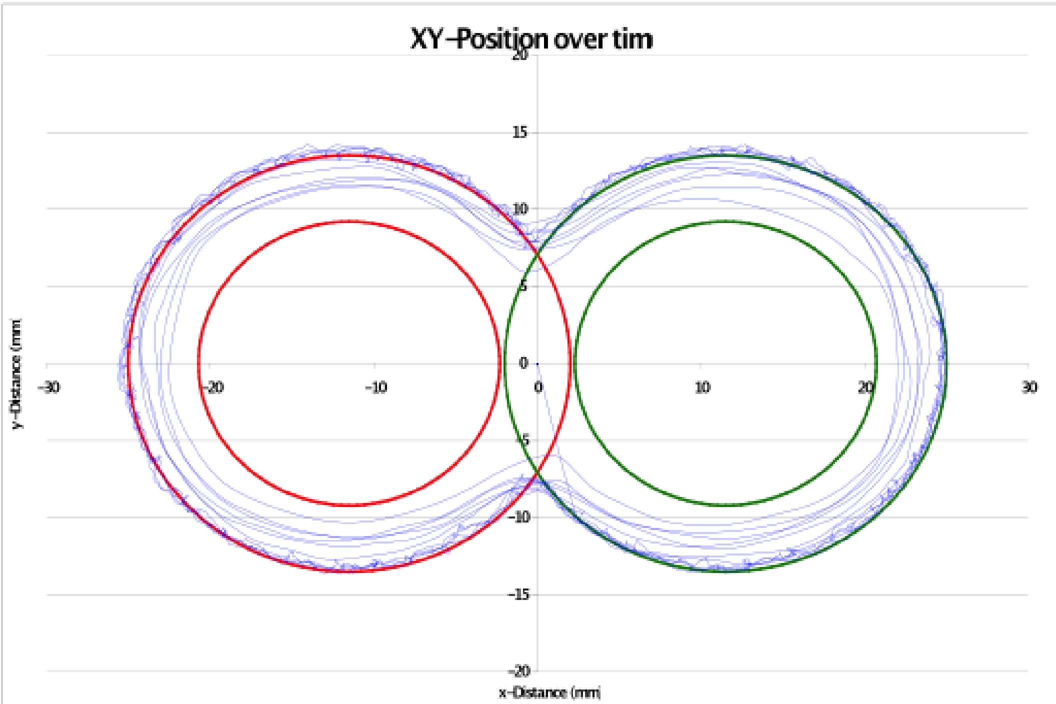


Figure 6-1-4: Flow path of a particle stuck in the melt film.

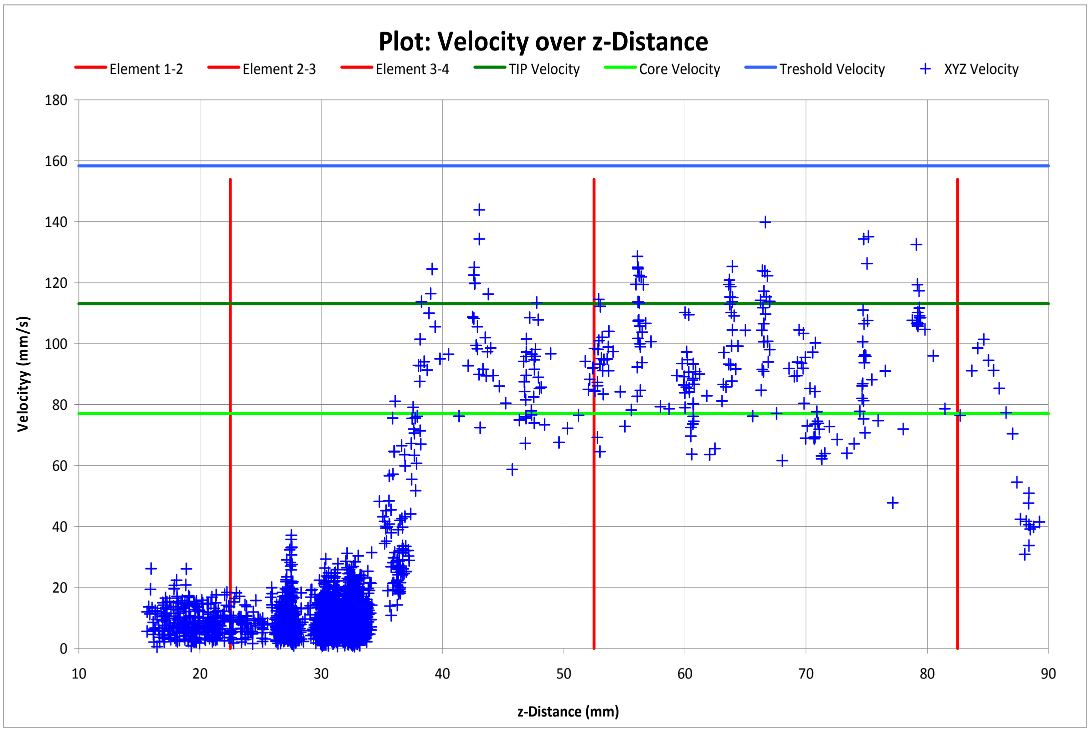


Figure 6-1-5: Velocity profile of a particle stuck in the melt film.

In the velocity profile illustrated in figure 6-1-5 it can furthermore be seen, that the speed of the particle was in the range of 10mm/s while it was moving through almost half of the first element. There were 2-3 incidents where the velocity was slightly higher and the particle was not far from being re-fed into the main material stream. This was most probably the case when a screw tip was passing.

Then at a z-value of about 35 mm the particle was suddenly washed away from the barrel surface and accelerated back to normal particle speeds of about 100 mm/s).

Such a flow condition can again be a problem with very temperature sensitive materials or in reactive processing, where narrow residence time distributions are needed.

7 The PEPT centre of Excellence

PEPTFlow has proven to be a unique tool for flow characterisation in TSE. The consortium will therefore leave the PEPTFlow TSE visualisation centre operational for at least 3 month after the end of the PEPTFlow project to offer this new characterisation technology to interested third parties.

During all 2009 training sessions this possibility was advertised to the attending compounders and some interest was noticed.

The following section gives a brief overview of the technical possiblities in this PEPTFlow imaging centre in Birmingham.

7.1 The University of Birmingham

The University of Birmingham was founded in 1900 and grew out of the radical vision of its first Chancellor, Joseph Chamberlain. He founded the University to create a new model for higher education and to produce the minds that would shape the modern industrial world. It was established by Royal Charter in 1900 and was the UK's first civic university. The first phase of building work on the campus was completed in 1909, making this year the centenary of the opening of the University.

Each year, over 4,000 students from 150 countries study at the University of Birmingham, enhancing its reputation as a truly international university, and adding to the diverse range of cultures, views and opinions. In addition to this around 23% of the academic staff are overseas nationals.

7.2 The PEPTFlow Centre

Within the University the **School of Physics and Astronomy** and the **School of Chemical Engineering** have developed the technique of (PET) and (PEPT), and the examination of the inner workings, of a twin screw plastics compounder, have been undertaken within the **School of Chemical Engineering.**

7.2.1 The Extruder

The extruder installed in the lab in Birmingham is a standard labscale TwinScrew extruder, a Leistritz Micro 27. The technical details are summarised in the table 7-2-1 below

Type of extruder	**Co-rotating Twin Screw Extruder (TSE)**	**Unit**
Screw diameter	27	mm
Screw length	36 D	
Number of barrel segments	9	
Max. Temperature Set-Point	400	°C
Max. Screw-Speed	400	1/min
Max. Melt pressure	250	Bar
Heaters	Electrical	
Cooling	Water	

Table 7-2-1: Technical details of the Leistritz 27mm Extruder

7.2.2 The Flexibility

The flexibility is a key factor in using TSE in compounding. The labscale extruder installed in Birmingham in principal offers the same flexibility in barrel and screw configuration standard machines offer as well. There are only some limitations that derive from the PEPT-Camera-System installed surrounding the extruder:

1. The PEPT-Window is currently installed in the barrel block number 7 (see figure 7-2-1)

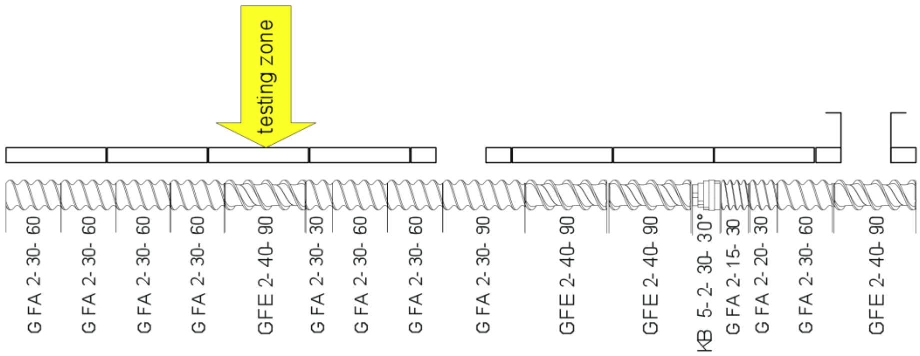


Figure 7-2-1: Standard position of the PEPT-Window.

Due to geometrical limitations in the movement of the camera system this PEPT-Window can only be moved to blocks 6 or 8.

2. The PEPT-Window is a special barrel block, that is manufactured from a high grade aluminium (see figure 7-2-2)

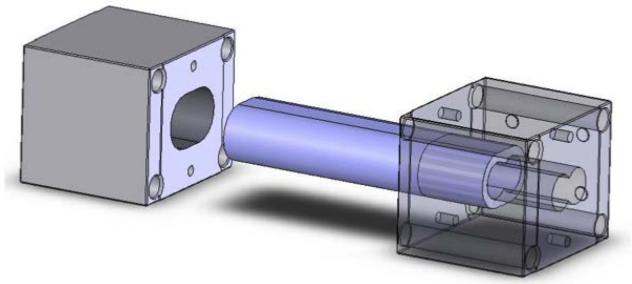


Figure 7-2-2: Inline for the PEPT-Window

There is a certain risk that the different thermal conductivity of aluminium and the missing heating and cooling in this window can have a less than minimal effect on the processing. Furthermore the processing of highly abrasive compounds will be difficult due to the reduced wear resistance of this extruder barrel element.

3. There is currently no degassing on the machine. It could be possible to install a vacuum dome on the machine, but it should be considered that the PEPT-Window is currently in the position of the typical degassing zone.
4. Side feeding is possible
5. Gravimetric as well as volumetric feeders could be supplied for the trials by the RTD partners Birmingham, Rapra and ICT.
6. Beside these limitations in the barrel configuration the screw is perfectly flexible in it’s configuration.
7. Any missing auxiliary equipment, like feeder, pumps, side feeders, and additional pelletizer could be supplied be the RTD partners upon request. Furthermore it is possible to provide this equipment by the interested third party as well.

7.2.3 The camera

Building upon the knowledge, obtained from the development of (PET) and (PEPT) at the University of Birmingham, the PeptFlow project has developed the all-enveloping camera system that is shown in the following two illustrations. This enables a full 360° view of the extruder to be monitored, thus giving the ability to track the motion of the polymer throughout the journey down the screw. This system is a valuable addition to the **Positron Imaging Centre**.

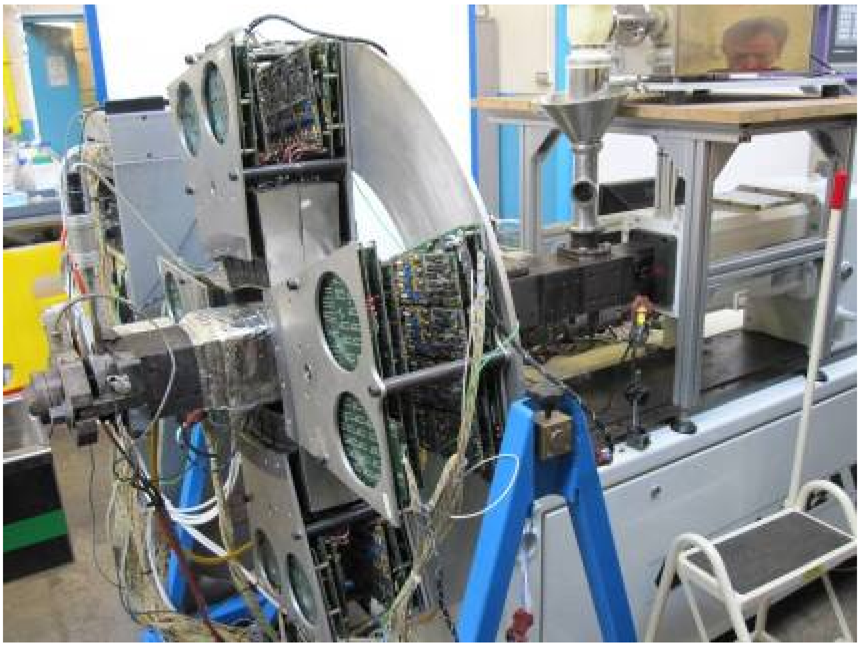


Figure 7-2-3: The camera system installed on the Leistritz 27mm Extruder

The knowledge gained from the PeptFlow project also extends to the ability to run a complete polymer processing operation where the polymer is compounded with other ingredients, and then pelletized into a form that can then be used in other processes such as injection moulding, blow moulding etc.

The team involved in operating PeptFlow at the University of Birmingham are therefore ideally placed to continue as the centre of excellence for Positron Emission Particle Tracking, with special reference to polymer processing.

Figure 7-2-4: The downstream equipment (water bath and pelletizer)

The illustration shows the downstream element of the compounding process, and some of the PeptFlow project team operating the line.

The potential and limitations of the currently installed camera system can be described as:

- Position frequency of up to 100 positions per second possible. This results in substantial distance between two tracer fixings. This is illustrated in the following table

Screw speed	Tip velocity	Distance between position fixes
1/min	mm/s	mm
50	70,69	0,71
100	141,37	1,41
150	212,06	2,12
200	282,74	2,83
250	353,43	3,53
300	424,12	4,24
350	494,80	4,95
400	565,49	5,65

- Due to the way the tracer is currently produced it seems to be very unstable in humid condition. Therefore it currently seems to be a problem to monitor materials with substantial amounts of humidity (fillers, hydroscopic polymers)

- Due to geometrical limitations the camera can only be mounted in the area without machine bed. Therefore monitoring is limited to the end of the extruder. This limitation might be possible to work around with some extra effort in reconfiguring the extruder engine setup.

7.2.3.1 Contact points

The central contact point at the University of Birmingham is:

Andy Ingram

Tel: +44 121 414 4548

e-mail: a.ingram@bham.ac.uk

7.2.3.2 Costs

The cost is negotiable on a case-by-case basis up to £2000 per day for standalone studies. This will include Tracer Production, Camera Operation, PEPT Study and Initial Analysis of Data. One day of PEPT would be expected to generate up to 50 particle trajectories assuming that significant process changes are avoided during the course of the run.

Birmingham University and the consortium is also interested in detailed collaborative project work.”

8 References

1. ‘Optimisation of Compounding Machines’, J.Colbert, Baker Perkins Chemical Machinery, ANTEC 1988.