February 1, 2006 SCO (Shirai Consulting Office) T. Shirai E-mail: <u>t_shirai@mvf.biglobe.ne.jp</u>

Abstracts of Polymer Processing Articles

Chapter 1. Flow Characteristics of Viscous Liquid

[Simulation Analysis for Polymer Processing by PC (1), Japan Plastics, Vol.49, No.11, P.86 (1998)]

When arguing phenomena of polymer processing, flow characteristics of polymer solutions or polymer melts are the most fundamental and important issues. Such flows are mostly laminar, and laminar flow is implicitly assumed throughout this series of articles.

Theoretical equations necessary for treating Newtonian fluid in which shear stress is proportional to shear rate, are presented first.

Most of all polymer fluids actually show non-Newtonian characteristics when considering some wide range of shear rate, and it often becomes important to treat polymer fluids as non-Newtonian in polymer processing.

Then, several non-Newtonian models, end correction method to get correct viscosity from experimental data, temperature dependency of polymer melt, empirical equation that can include both temperature and shear rate dependencies, and other important matters are explained.

Chapter 2. Flow in Sheeting Die

[Simulation Analysis for Polymer Processing by PC (2), Japan Plastics, Vol.49, No.12, P.86 (1998)]

As an example of analytical treatment of non-Newtonian flow, flow in sheeting die, such as T die and coat hanger die, is taken up. To be concrete, thickness distribution, pressure drop, die lip adjustment to attain even thickness of film are discussed.

Among theories of sheeting die, a useful theory by McKelvey et al. [1] treats the fluid as isothermal power law. Before this theory, there were some

^{*} This collection of abstracts is written in English, but original articles are written in Japanese.

theories of non-Newtonian flow in sheeting die, but they adopted rather simple die shapes or dimensions.

In contrast, the theory of McKelvey et al. can be used when analyzing more complicated sheeting dies, and can apply to practical cases.

[1] McKelvey, J. M. et al, Polym. Eng. & Sci., 11 (3), 258 ('71)

Chapter 3. Heating/Cooling of Solid

[Simulation Analysis for Polymer Processing by PC (3), Japan Plastics, Vol.50, No.1, P.147 (1999)]

Heating or cooling of rod or yarn can be taken as a matter of heat transfer of circular bar. In case of film or sheet, it can be considered as flat plate. Heat transfer analysis of circular bar or flat plate is rather simple, but it furnishes very useful knowledge when analyzing heat treatment process etc. of plastic rods or films.

In this chapter, theories, numerical analysis and computer programs on the above subjects are discussed in detail.

Chapter 4. Flow and Heat Transfer of Viscous Liquid in Tube

[Simulation Analysis for Polymer Processing by PC (3), Japan Plastics, Vol.50, No.1, P.147 (1999)]

To analyze flow and heat transfer of polymer fluid precisely, viscous heat generation and heat transfer of non-Newtonian fluid flow shall be considered. In such cases, heat transfer, internal heat generation, temperature and shear rate dependency of fluid viscosity are to be taken account. This level of analysis is worthy of saying "simulation".

Numerical method of getting temperature change, temperature distribution and pressure drop of non-Newtonian fluid in circular tube under constant surrounding temperature is discussed in this chapter. This is one of the most fundamental techniques of polymer processing analysis, and is simple but useful having high utilization.

This method will be a good reference when using similar technique, and is discussed in some detail here.

Chapter 5. Flow and Heat Transfer of Viscous Liquid in Slit

[Simulation Analysis for Polymer Processing by PC (4), Japan Plastics, Vol.50, No.2, P.86 (1999)]

Flow and heat transfer of fluid in slit can be solved by a similar method described in the previous chapter. In this chapter, flow in slit, including cases where temperatures of both walls are different, and the case of sliding wall, are discussed.

Analyzing flow and heat transfer in slit is also one of the fundamental techniques when analyzing polymer process, and is simple but useful.

Chapter 6. Melt Extruder (Newtonian Flow)

[Simulation Analysis for Polymer Processing by PC (4), Japan Plastics, Vol.50, No.2, P.86 (1999)]

Widely used screw extruders for polymer processing are plasticating extruders, where solid pellets or flakes are melted and pumped. Screw pumps that are used to transport viscous fluid, e.g. pumps for pulling out molten polymer from polymerization vessels, are also in practical use.

Melt conveying theories of screw extruder are discussed in this chapter and in the next. These theories can be applied to the analysis of metering zone of plasticating extruder too.

This chapter treats screw extrusion of Newtonian fluid.

Chapter 7. Melt Extruder (Non-Newtonian Flow)

[Simulation Analysis for Polymer Processing by PC (5), Japan Plastics, Vol.50, No.3, P.90 (1999)]

Newtonian extrusion theory given in the previous chapter is useful when calculating approx. performance of screw extruder, but non-Newtonian and non-isothermal analysis is necessary for more precise treatments. For example, when extruding high viscosity liquid, viscous heat generation can't be neglected and to know temperature change in extruders becomes very important. For this purpose, non-Newtonian and non-isothermal extrusion shall be considered.

Miscellaneous theories of non-Newtonian extrusion have been reported for a

long time. When trying to analyze more precisely, theory become more complex.

A sophisticated and practical one is Fenner's [2], [3] non-Newtonian and non-isothermal two-dimensional extrusion theory that takes account of both down channel and cross channel flows. In this chapter, the theory of Fenner and its numerical calculation method are described in detail.

- [2] Fenner, R.T., Polymer, 16, 293 ('75)
- [3] Fenner, R.T., 'Principles of Polymer Processing', P.109, Macmillan Press ('79)

Chapter 8. Plasticating Extruder (Tadmor Model)

[Simulation Analysis for Polymer Processing by PC (5), Japan Plastics, Vol.50, No.3, P.90 (1999)]

A plasticating extruder melts and extrudes fluid of plastics, through its three functions, i.e. solid conveying, melting (plasticating) and metering. Among these three functions, plasticating is the most important and complicated process.

Tadmor published the plasticating extruder theory [4.] first. This theory assumes the melted fluid as Newtonian, and does not necessarily match with experimental results well, but it becomes the foundation of the next non-Newtonian model and is important.

The Newtonian theory was followed by the famous non-Newtonian theory also by Tadmor et al. [5], [6]. This new model conforms to actual data fairly well. The theory was an epoch-making one in the sense of making possible to treat the plasticating process theoretically.

In this chapter, Newtonian Tadmor model is presented first, and then non-Newtonian model is described with detail explanation of its simulation program and a calculation example.

- [4] Tadmor, Z., Polym. Eng. & Sci., 6, 185 ('66)
- [5] Tadmor, Z. et al., Polym. Eng. & Sci., 7, 198 ('67)
- [6] Tadmor, Z. & Klein, I., 'Engineering Principles of Plasticating Extrusion', P.133, Van Nostrand Reinhold ('70)

Chapter 9. Plasticating Extruder (Donovan Model)

[Simulation Analysis for Polymer Processing by PC (6), Japan Plastics, Vol.50, No.4, P.122 (1999)]

After Tadmor model was published, many theoretical models of plasticating extrusion have been made public. Among them, Donovan model improves Tadmor model substantially.

Tadmor model assumes that the solid bed velocity in down channel direction (z) is constant, and the thickness of the solid bed is infinite as for heat transfer. On the contrally Donovan model [7] allows the solid bed to accelerate during melting by introducing SBAP (solid bed acceleration parameter), and takes into account the heat transfer from the screw by dealing the solid bed with finite thickness.

In this chapter, theory of Donovan model is explained by contrasting with Tadmor model, and a calculation example using Donovan model is shown as well.

[7] Donovan, R. C., Polym. Eng. & Sci., 11 (3), 247 ('71)

Chapter 10. Solid Conveying in Extruder

[Simulation Analysis for Polymer Processing by PC (6), Japan Plastics, Vol.50, No.4, P.122 (1999)]

Different theoretical treatments shall be applied to solid conveying extruder or solid conveying zone of a plasticationg extruder, from melt conveying zone. Usually solid conveying theories assumes that the plastics pellets move in the screw channel as unified solid plug, and shall consider screw geometry, number of revolution, friction coefficients of the solid plug with barrel surface and screw surface, and pressure gradient.

Darnell & Mol first published solid conveying theory of extruder [8]. This theory assumes both of the friction coefficients of the solid plug with barrel and screw are same, and neglects flight width of the screw. Later on, Tadmor et al. presented an improved theory [9].

This chapter describes the above theory by Tadmor et al., and then shows a calculation example using the theory.

- [8] Darnell, W. H. & Mol, E. A. J., SPE J., 12, 20 (April,'56)
- [9] Tadmor, Z. & Klein, I., 'Engineering Principles of Plasticating Extrusion', P.55, Van Nostrand Reinhold ('70)

Chapter 11. Screen Filter

[Simulation Analysis for Polymer Processing by PC (7), Japan Plastics, Vol.50, No.5, P.96 (1999)]

For the purpose of filtration and gel dispersion, screen filters are frequently used in polymer processing. Screen filters for these purposes are mostly combinations of multiple different mesh screens.

Carley et al. published calculation method [10] for this type of screen filter. This theory is for isothermal non-Newtonian fluid.

This chapter presents the theory and its calculation example.

[10] Carley, J. M. & Smith, W. C., Polym. Eng. & Sci., 18 (5), 408 ('78)

Chapter 12 & 13. Flow in Spiral Die (1) & (2)

[Simulation Analysis for Polymer Processing by PC (7), Japan Plastics, Vol.50, No.5, P.96 (1999) & Simulation Analysis for Polymer Processing by PC (8), Japan Plastics, Vol.50, No.6, P.120 (1999)]

Spiral dies, which have built-in mandrels with spiral grooves, are frequently used to produce uniform films and sheets.

The flow inside this type of die is a combination of flow in the groove direction and flow toward the die exit. The purposes of using spiral die are to attain improved mixing and uniform flow rate circumferentially, during polymer melt flows in the spiral groove and across the flight clearance in complicated manner.

Procter presented a flow theory in a spiral die [11], but it is based on considerable simplifications. Here presents more sound theory, which was extended by the present writer, starting from Procter's.

In chapter 12, the extended theory, simulation program using the theory and a calculation example are described in detail, in terms of flow and pressure drop in the spiral die.

In chapter 13, theory to evaluate degree of mixing is presented, and at the

end, a practical example of investigating the structure of the die, using the methods given in chapter 12 and chapter 13.

[11] Procter, B., SPE J., 28, 34 (Feb.,'72)

Chapter 14 & 15. Film Blowing (1) & (2)

[Simulation Analysis for Polymer Processing by PC (8), Japan Plastics, Vol.50, No.6, P.120 (1999) & Simulation Analysis for Polymer Processing by PC (9), Japan Plastics, Vol.50, No.7, P.86 (1999)]

Film blowing, which is a typical film manufacturing process, is widely applied to many kinds of plastics.

Chapter 14 presents the most fundamental theory by Petrie [12] who is a noted researcher of this field, and describes the method of analytical calculation, simulation program and a calculation example using the theory. This theory treats the polymer flow as non-isothermal Newtonian.

One of the issues of the theory given in chapter 14 is the assumption of linear temperature gradient while cooling the brown film without introducing heat balance. Kanai et al. published an improved theory [13] in terms of this issue.

In chapter 15, this improved theory and simulation program based on the theory are explained.

[12] Petrie, C. J. S., A I Ch E J., 21 (2), 275 ('75)
[13] T. Kanai, White, J. L. et al., Sen-i Gakkaishi, 40 (12), T-465 ('84)

Chapter 16. Calendering

[Simulation Analysis for Polymer Processing by PC (9), Japan Plastics, Vol.50, No.7, P.86 (1999)]

Calendering is a process of producing sheets with uniform thickness, by passing soften or molten plastics material, through a nip clearance of two rotating rolls.

McKelvey published the most fundamental theory [14], [15] which assumes the fluid is Newtonian, laminar, isothermal and incompressible. And also assumes the clearance between rolls is small compared with the radius of the roll, and therefore the gap between rolls gradually changes when approaching the nip point.

This chapter describes the above-mentioned theory, and presents simulation program to analyze fluctuation of product thickness and its calculation example.

- [14] McKelvey, J. M., 'Polymer Processing', P.211, John Wiley & Sons ('62)
- [15] Tadmor, Z. & Gogos, C. G., 'Principles of Polymer Processing', P.363, John Wiley & Sons ('79)

Chapter 17. Coater Dryer

[Simulation Analysis for Polymer Processing by PC (10), Japan Plastics, Vol.50, No.8, P.95 (1999)]

Film coating is an important process for film processing, where polymer-solvent solution is coated on plastics films etc., and continuously passing through dryer(s) the solvent is evaporated.

The coating process is applied to the production of adhesive tapes, photo-films, wrapping films, magnetic tapes, dry film resist (DFR) used for producing printed circuit boards, etc.

To analyze the drying process of the coated film, it is necessary to consider heat transfer in the base film and the coated film (solution layer) together, and mass transfer in the coated film accompanying evaporation of the solvent at the surface. It could be said this is a complicating and interesting problem.

In this chapter, theoretical equations derived by the present writer referring to the theory of dry spinning [16], simulation program based on the theory and its calculation example are presented.

[16] Ohsawa. Y. et al., J. Appl. Polym. Sci., 14, 1879 ('70), etc.

Chapter 19. Film Casting

[Simulation Analysis for Polymer Processing by PC (11), Japan Plastics, Vol.50, No.10, P.105 (1999)]

Theories about the behavior of film deformation from the exit of a flat

sheeting die to a take-up roll, had been made public little if anything. Kanai published a theory [17] that can simulate temperature, velocity, thickness, strain rate, stress etc. during the film running downward.

Similarity between this theory and the theory of melt spinning is high, so the present writer developed Kanai's equations to the level of adopting the same procedure for solving the melt spinning equations.

This chapter presents Kanai's theory and equations together with the developed ones, and a calculation example using these equations.

[17] T. Kanai, Sen-i Gakkaishi, 41 (10) T-409 ('85)

Chapter 20. Scale-up Rules of Extruder

[Simulation Analysis for Polymer Processing by PC (11), Japan Plastics, Vol.50, No.10, P.105 (1999)]

At the last chapter of this series, scale-up rules of extruder are taken up. Scale up rule cannot bring out equivalent answer by simulation, but is used frequently as a simple method of guessing approximate answer from the data of small-scale equipment.

Many scale-up rules of extruder have long been published. Most of all rules focus on the behavior of melt, and the basic premise of the scale up is getting same quality (mixing degree) and temperature of the melt.

This chapter presents miscellaneous scale-up rules [18], [19], [20], [21], including a rule claiming for getting same quality of plasticating extruder [22], and their calculation examples.

- [18] Maddock, B. H., Polym. Eng. & Sci., 14 (12), 853 ('74)
- [19] Rao, N. S., 'Designing Machines and Dies for Polymer Processing with Computer Programs', P.120, Hanser ('81)
- [20] Fisher, P., SPE ANTEC, Vol.23, P.464 ('77)
- [21] M. Yoshida, Technical Bulletin of Japan Steel Works, No.28, P.37
- [22] Lutterbeck, J. et al, SPE ANTEC ('82)

Computer Simulation of Plasticating Extruder by Chung Model

[Computer Simulation of Plasticating Extruder by Chung Model, Japan Plastics (July extra

issue), P.156 (2005)]

A unique melting model of an extruder has been developed based on experimental results by a simulative apparatus called "screw simulator" and theoretical studies on them, by Mount, Chung et al. There were discussions about the adequacy of applying the knowledge from the screw simulator to real single screw extruders. Chung and coworkers persevered in their research, and published their achievements in book form [23] in 2000. In this book, not only melting zone but also other zones, i.e. solid convey zones etc., of plasticating extruders are comprehensively discussed in detail, from unique point of view. But simulation procedure using Chung model is not mentioned specifically.

The present writer developed a computer program, which simulates the melting process of a plasticating extruder using the model. The simulation program seems to give reasonable results judging from some trial calculations.

In this article, theory of Chung model, its simulation program, and calculation examples are described in detail.

[23] Chung, C. I., 'Extrusion of Polymers: Theory and Practice', Hanser Publishers, Munich (2000)

Computer Simulation of Coater Dryer (Part 1) & (Part 2)

[Computer Simulation of Coater Dryer (Part 1), Japan Plastics, Vol.56, No.12, P.90 (2005) & Computer Simulation of Coater Dryer (Part 2), Japan Plastics, Vol.57, No.1, P.175 (2006)] Film coating is an important process for film processing, where polymer-solvent solution is coated on plastics films etc., and continuously passing through dryer(s) the solvent is evaporated.

The coating process is applied to the production of adhesive tapes, photo-films, wrapping films, magnetic tapes, dry film resist (DFR) used for producing printed circuit boards, etc.

To analyze the drying process of the coated film, it is necessary to consider heat transfer in the base film and the coated film (solution layer) together, and mass transfer in the coated film accompanying evaporation of the solvent at the surface. It could be said this is a complicating and interesting problem. The present writer already published an article about drying in a coater dryer (its abstract is included in this collection of abstracts). Important difference of the present article from the previous one is the method of obtaining the diffusion coefficient in coating liquid. The diffusion coefficient is one of the most important factors that control the drying process.

In short, the diffusion coefficient is decided by fitting experimental data, in the previous model. Contrary to the previous model, the diffusion coefficient is derived by calculation using physical properties in the present model. Namely, no experimental data is necessary to simulate the drying process, but depending on the circumstances, getting all necessary physical properties is quite difficult.

From practical point of view, both of these two models have advantages and disadvantages, and using these models on a case-by-case basis will be wise.

To calculate the diffusion coefficient, Vrentas-Duda free volume theory [24], [25] is adopted in the present model.

In this chapter, theoretical equations, simulation program based on the present model and its calculation example are presented, mentioning the previous model.

- [24] Duda, J. L., Vrentas, J. S., Ju, S. T. and Liu, H. T., AIChE J., 28 (2), 279 ('82)
- [25] Zielinski, J. M. and Duda, J. L., AIChE J., 38 (3), 405 ('92)