

Modelling in Applied Physics: The Case of Polymers

*Towfic L. Shomar **

ABSTRACT

Until recently philosophy of physics has been overshadowed by the idea that the important philosophical issues that can be derived from physics are related only to fundamental theories, such as quantum mechanics and relativity. Applied fields of physics were deemed as unimportant. The argument for such a position lays in thinking that these applied fields of physics depend in their theoretical representations on fundamental theories and hence are reducible to these fundamental theories. It would be hard to defend such a position, keeping in mind that applied fields of physics have a life of its own totally separate from fundamental physics and have in fact a lot to say to philosophers.

The field of polymers is one of the branches of applied physics that has a lot to say to philosophers. It is a field of physics where theoreticians failed to present a coherent theory that can capture the different ways polymers can be built. This paper examines the difficulties that keep theoreticians away from having such a theory, revealing what kind of philosophical lessons polymers might have.

The main thesis is: even in the cases where a theory predicts the possibility of developing a specific type of polymers that was not previously known, the exact model that represents the outcome polymer theoretically will not be even in principle derivable from the theory that predicted its existence in the first place.

KEYWORDS: Models, theoretical models, phenomenological models, model construction, polymers, representation, and philosophy of physics.

1. INTRODUCTION

For many years now, it has been pointed out that models in physics are produced in two distinct ways. These are theoretical models: that is, models built from a top-down strategy; and the other is built on a bottom-up strategy, these are phenomenological models.

In earlier works of Shomar (2000); Shomar (1998); Cartwright, Shomar and Suarez, (1995), examples from superconductivity were utilized to demonstrate that phenomenological models are better representation of nature than models derived from fundamental theories (i.e. theoretical models). A claim was forwarded stipulating that if a realist position is to be viable, consistent and capable of overcoming the deep criticism of both the pessimistic meta-induction (Laudan, 1981)

and empiricism (Van Fraassen, 1980), it ought to be built on the assumption that only phenomenological models are the true representative of nature while “fundamental” theories and theoretical models are mere tools.

In the examples from superconductivity, the idea was that the models are built from a bottom-up approach and there is no direct way of deriving these models from fundamental theories. Moreover, these models are in direct contradiction with the fundamental theories due to additional parameters that are introduced into them. Nonetheless, they are more capable of explaining and representing the physical phenomena they were meant to model.¹

Recent works in modelling in physics and economics provide a good base to look at models from a different perspective. Nancy Cartwright’s concept of models as the

* Assistant Prof., Philadelphia University, Jordan, Research Associate, CPNSS, LSE, London. Received on 11/9/2005 and Accepted for Publication on 9/5/2006.

¹ This paper concentrates on the idea of models ability of representing the phenomenon. Whether these models are capable of predicting or not is an interesting question, but such a question goes beyond the scope of this paper.

blueprints of nomological machines (Cartwright, 1999:180) and Margaret Morrison's concept of models as mediators (Morrison, 1997), are only part of what may be called "The London School" in philosophy of science, which looks at theories as mere tools that can be used to build different kinds of models: phenomenological and theoretical. Other writers² expressed different angles of the discussions on models that took place at the London School of Economics between 1993 and 1997, a number of which were alluded to in "Models as Mediators" (Morrison and Morgan, 1999).

Keeping this tradition in mind, a stronger claim will be argued here where it will be demonstrated with an example from polymers that even if the polymeric structure itself and its specifications were suggested by a certain theory incorporating a model of that polymeric structure, i.e., even in the cases where a theory predicts the possibility of developing a specific type of polymers that was not previously known, the exact model that represents the outcome polymer theoretically will not be, even in principle, derivable from the theory that predicted its existence. In this paper, liquid polymers and their dynamics will be concentrated upon.

As we all know, physicists do not draw any philosophical distinctions when dealing with a physics problem. They would only care for certain boundaries and redlines that they ought not to cross. Maybe at a later stage, i.e. after arriving to what they would agree on as a good representation of the problem and its solution, they might start to think of the philosophical implications of these representations. Recently, in a more elaborate view, physicists are starting to be puzzled by the great difference between the simplicity of the laws of physics and the complexity of the real phenomena these laws claim to capture. One of these expressions of such puzzling experience has recently been published in *Science* (Goldenfeld and Kadanoff, 1999). It revisits, in a way, the same questions P. Anderson tried to answer thirty years ago. The idea is simple; the complex structures of physics and nature obey different laws from those of the sub-structures that build these complex structures. Hence, "More is Different" (Anderson, 1972).

In the context of polymers, Kröger stresses in a recent review paper of the currently accepted models on polymers that:

"Physical phenomena occurring in complex materials cannot be encapsulated within a single numerical

paradigm. In fact, they should be described within hierarchical, multi-level numerical models in which each sub-model is responsible for different spatio-temporal behaviour and passes out the averaged parameters to the model, which is next in the hierarchy" (Kroger, 2004:454).

In such cases, these different models are not, and cannot be, reducible to one theory but they take their tools from different theories.

2. POLYMERS, THE BASICS

Polymers are chains of repetitive simple molecules that would end up appearing as a one macromolecule. These chains would obey the simple mechanisms of molecules if they continue to operate on a one-dimensional level, i.e. when the polymeric chain would be a linear chain. Most polymers operate on more than one dimension. The moment that a node exists between any two chains, or within the same chain, the resulting polymeric chain would be three-dimensional. Polymers are of two kinds with many variations of types within. These are natural polymers, i.e. polymers that are in nature without human intervention, such as the DNA, proteins, etc., and man made polymers³. The second kind consists of many types of structures that are manipulated inside laboratories and within industry. We can say that different processing conditions determine the difference between protein and high strength polymer fibres, i.e. the human intervention is what makes these high polymers what they are, with their special properties that are arrived at through very careful and elaborate processes.

In general, the structure of polymers can be expressed on the phenomenological level by using very simple models that oversee either the underlying structure, or the mechanism behind the characteristic surface behaviour observed.

Treatment of polymers involves the adaptation of a number of concepts, which are imported from other areas of physics such as critical phenomena, liquid crystals and superconductors. In a way, physicists would use these concepts and models when they see some parallels between the behaviour of polymeric coils and chains with that of other areas in physics. These parallels involve statistical summations of directional vectors in thermally equilibrated systems and other simpler laws. Some of these

² M. Suarez, M. Boumans, M. Morrison and M. Del Seta.

³ There are many type of man made polymers to name but some: Star Polymer, Dendrimer, Stereoregular, isotactic, atactic, etc.

laws express a linear behaviour as is usually suggested by the “fundamental” theories of physics, such as:

- 1). Hookean Elastic $\sigma = E \gamma$
- 2). Newtonian Fluid $\tau = \eta (d\gamma/dt) = \eta (dv_x/dy)$, where τ is the shear stress
- 3). Fourier's Law $q_y = -k (dT/dy)$
- 4). Fick's Law $J_{Ay} = -D_{AB} (dc_a/dy)$

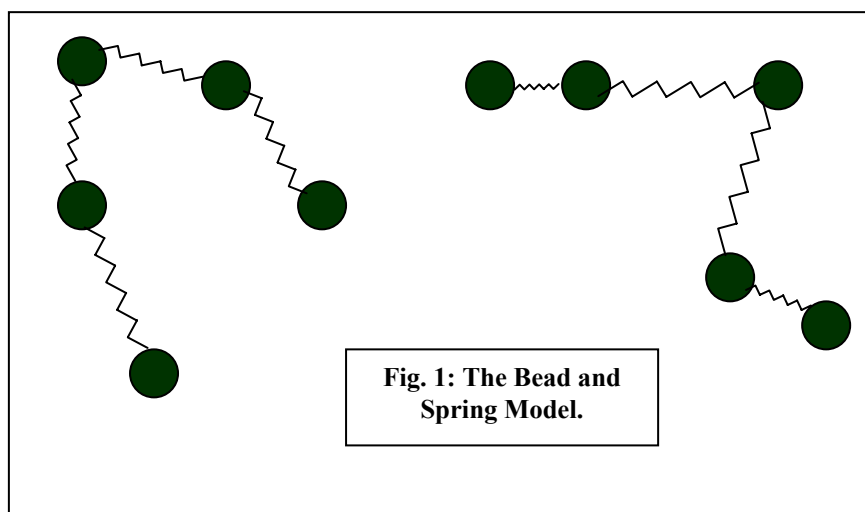
Such laws might be good approximations on the macro-level but they do not help us to understand why such phenomena occur. To understand that it would need a deeper look into the sub-structure of polymers.

Consider the two mechanisms given by the linear laws 1 and 2: the Hookean elastic that reflects ideal solids and the Newtonian fluid that reflects liquid behaviour. These two are ideal equations expressing the differences in two ideal mechanisms in response to perturbation. The Hookean elastic is imported from mechanics to describe polymers behaviour of not absorbing energy in deformation; by using such law, polymers’ physicists were able to develop a simple molecular model that asserts that, under stress, atoms are displaced from their equilibrium positions and return to these positions upon release of the stress, exactly as the case in strings. In the case of Newtonian fluids, polymers completely absorb the energy of deformation,

which leads to the deployment of a simple model that describes the complete displacement of atoms after traversing an energy barrier associated with two equilibrium positions in the liquid.

Nonetheless, these two ideal models do not describe polymers in general when they are under mechanical perturbation, i.e., polymers do not display perfect Hookean behaviour in the solid state due to a high degree of disorder in their structure, which results from their complexity when compared with a simple metallic crystal, for instance. Hence, energy is always lost in deformation of a solid polymer. In addition, polymers do not display perfect Newtonian behaviour, for similar reasons, i.e., atomic motions in polymeric liquids are coupled due to the chain like nature, and there is a wide dispersion of energy states in these disordered liquids.

Hookean behaviour is expressed by what is known as “the Bead and Spring Model” for a chain. Such a model is derived regardless of the type of polymer lattice. This model is useful in estimating the kinetic features of ideal coils such as the viscosity of Gaussian polymer chains. It considers a chain composed of balls connected by Hookean springs, where the distribution of the springs and bonds follow a Gaussian distribution. (See the figure below.)



Even if the models that represent polymeric structure would vary due to the level that it represents, i.e. micro or macro level, this distinction is a matter of arbitrary cut-off as Gorban et al. (2001) tell us:

“Division into ‘micro’ and ‘macro’ is context-dependent: what is regarded as ‘micro’ in one statement of the problem can become ‘macro’ in a different context.”

They continue to say that:

“In view of many possible paths from micro to macro, any reasonable procedure of coarse-graining the evolution equation should satisfy the following requirement of commutativity of diagrams:

$$\Pi_{2 \rightarrow 3} + \Pi_{1 \rightarrow 2} = \Pi_{1 \rightarrow 3} \quad (1)$$

Here, 1, 2, and 3 are different levels of description, and $\Pi_{i \rightarrow j}$ transforms from a microscopic level of description to a more macroscopic level. The diagram must be commutative: it should not matter as to which route of coarse-graining was taken to come from microscopic level 1 to macroscopic level 3. One route (1 \rightarrow 2 \rightarrow 3) goes stepwise, first to some intermediate level 2 and then from level 2 to level 3." (Gorban et al., 2001:206).

This would mean that there should be some kind of translation between each level and the next level in order to ensure that the mathematical relations would in fact map the natural continuity between these levels. However, most of the theoretical descriptions of modern polymer theoretical representations are based on an understanding and description of fluctuations. This is a common way to describe random systems with statistical features. In such cases, fluctuations with a certain wave number ought to be looked at independently of any other fluctuations.

The real features of liquid polymers vary from Newtonian liquids in the following ways⁴:

- 1) While descending freely from a hall, Newtonian liquids stream down losing thickness, while liquid polymers widen 3 times the hall size.
- 2) A Newtonian liquid in a cylinder with a rotating rod shows a vortex, while a polymer liquid climbs the rod.
- 3) While flowing down an inclined tunnel, a Newtonian liquid assumes a flat surface, while the polymer liquid shows a convex surface.
- 4) While moving vertically from a wide cylinder to a narrow one, a Newtonian liquid exhibits straight and directed velocity fields, while a polymer liquid exhibits a large toroidal vortex.
- 5) Cutting a thick polymer liquid being poured demonstrates that the part below the cut obeys gravity while the part above the cut returns to the original container, in direct contradiction with a Newtonian liquid behaviour.

Considering all these elements, would it be possible to find a generalised (Newtonian) theory of any kind in polymers? Well, many polymer physics books would tell us that there are many generalisations that can be established concerning polymers. The laws that have been pointed out earlier belong to one of these generalisations. In the next section, one other type of generalisation will be discussed: the construction of a non-Newtonian fluid model.

One other attempt to introduce a general equation modelling stress differences in terms of the rate of strain was first introduced by Criminale-Ericksen-Filbey, the derivation of which was by no means conventional. The equation is:

$$\tau = -\eta \dot{\gamma} - \left(\frac{1}{2} \Psi_1 + \Psi_2 \right) \left\{ \dot{\gamma} \cdot \dot{\gamma} \right\} + \frac{1}{2} \Psi_1 \frac{D \dot{\gamma}}{Dt} \quad (2)$$

The first part

$$-\eta \dot{\gamma} - \left(\frac{1}{2} \Psi_1 + \Psi_2 \right) \left\{ \dot{\gamma} \cdot \dot{\gamma} \right\},$$

represents Generalised Newtonian Fluids. The second part $\frac{1}{2} \Psi_1 \frac{D \dot{\gamma}}{Dt}$, describes constitutive equations, which is

parallel to the Generalised Newtonian equation for normal forces. This "generalised" equation has several manifestations, which are:

1. Power-Law Fluid:

$$\eta (d\gamma/dt) = m (d\gamma/dt)^{n-1} \quad (3)$$

The n-1 power is a direct consequence of the first term in equation (2). This is a power-law equation for high strain rates. This kind of model is an empirical equation of 2 empirical parameters.

2. Ellis Model: this model (and the next) describes the knee part of the strain rate curve for viscosity, and uses 3 empirical parameters:

$$\eta_0 / \eta(t) = 1 + (\tau / \tau_{1/2})^{\alpha-1} \quad (4)$$

where η_0 is the zero shear rate viscosity and $\tau_{1/2}$ is the value of τ .

3. Carreau Model: this model uses 4 empirical parameters

$$\frac{\eta(j) - \eta_\alpha}{\eta_0 - \eta_\alpha} = \left\{ 1 - (\gamma_j)^2 \right\}^{(\alpha-1)/2} \quad (5)$$

Where η_0 is the solvent viscosity for solutions or zero for polymer melts.

4. Bingham Fluid: this model is used for fluids that display a solid like behaviour:

$$\eta(j) = \eta_0 + \frac{\tau_y}{j} \quad (6)$$

5. Constitutive Equations for Normal Forces: this model is used in the case of a steady flow in a tube:

$$\begin{aligned} \Psi_1 &= \Psi_1 j^2 \\ \Psi_2 &= \Psi_2 j^2 \end{aligned} \quad (7)$$

As we can see here, even in the case of a simple model, when suggesting a generalisation that might be

⁴ For illustrated photos of such differences see the following web page: <http://www.eng.uc.edu/~gbeaucag/classes/processing/chapter3.html>

counted as a good generalisation for polymeric structure, we discover many elements: the derivation is not conventional; the generalised form has more than one type; each of which is applied upon certain boundary conditions; and many parameters set in these sub-models are what are known as empirical parameters⁵.

One other point might be added at the end of this much skimmed pass over the basics of polymers is the fact that many of the elementary models that express the macroscopic properties of polymers deal with end-to-end behaviour, regardless of what would happen in between. In a way this is an approximation that is suggested for simplicity, because the microstructure is complex and problematic, and due to the fact that the macro-behaviour of these sub-structures would act similarly, it is possible, for practical reasons to assume that it is important to look at the end-to-end behaviour rather than the path behaviour.

Some might say it would be sufficient to capture the phenomenon so long as we can understand it, but for many physicists this would not be enough. Because understanding the path behaviour is what helps them in developing the processes for industrial applications requiring better polymer structures that are more suitable for the intended industrial applications, or yet new structures that are more appropriate for humans. Hence, it is essential to be able to understand the path behaviour as well as the end-to-end behaviour. This would lead us directly to the next section of this paper: the way one of the path behaviour models on the micro and mesoscopic level is constructed.

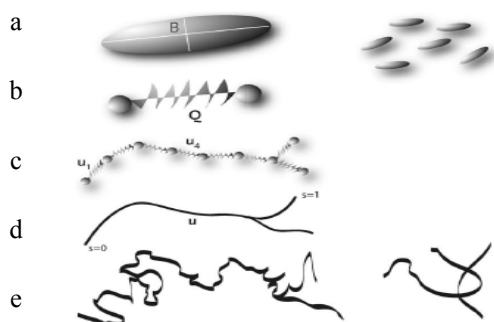


Fig. 2 “Simple microscopic models for complex Fluids with increasing level of abstraction and decreasing degrees of freedom (lhs, bottom to top), and their sketched range of application: (a) atomistically detailed polymer which accounts for anisotropic intermolecular interactions including entanglements, (b) coarse grained model via a mapping to a ‘primitive path’, (c) further approximated by

a multi-bead (nonlinear FENE) chain, (d) further coarse-grained to a (FENE) dumbbell which accounts for entropic elasticity and orientation but not for entanglement effects, and (e) ellipsoids of revolution including rigid rods, dissipative particles, with spherical or mean-field interaction. Models must meet the requirement of being thermodynamically admissible (Kröger, 2004: 459).

3. NON-NEWTONIAN MODEL

In the second and third levels (micro and mesoscopic) mentioned above, the Generalised Newtonian Fluid model with all its variations would not be able to describe the polymeric behaviour. In such cases, a non-Newtonian model is constructed. This is the Finitely Extendable Non-linear Elastic (FENE) chain model⁶, a dynamic model that operates on non-Newtonian rheology fluids, depending on the kinetic theory of fluids.

In such non-Newtonian fluid, known as viscoelastic fluid in confined geometry (Kröger, 2004)⁷, the governing conservation laws are:

$$\rho \frac{Dv}{Dt} = \nabla \cdot (-pI + \tau), \quad (8 \text{ and } 9)$$

$$\nabla \cdot V = 0$$

where ρ is the density, p is the pressure, v is the velocity field, I is the unit tensor, τ is the extra stress tensor and

$$\frac{Dv}{Dt} = \frac{\partial v}{\partial t} + v \cdot \nabla v$$

is the “material time” derivative (convective derivative).

Now if we start from the bead and spring models mentioned in section one, and take one section of these beads and springs (dumbbell), we would find that the maximum extensibility of the dumbbell is fixed at some value determined by the dimensionless parameter Q_0^2 and the spring force. After some scaling, this might take the form of:

$$F^{FENE} = - \frac{H}{1 - \frac{Q^2}{Q_0^2}} Q \quad (10)$$

⁶ The FENE model was first introduced by: (Warner, 1972).

⁷ For details of model construction see: (Halin et. al., 1998), Another example of the way FENE is used to construct models that describes polymer behavior appears in: (Lozinski and Chauviere, 2003).

⁵ For detailed discussions on basic physical properties of polymers consult: (Strobl, 1997) and (Doi and Edwards, 1986).

where H here is the harmonic spring coefficient. This is a “valid” approximation

“to a chain of freely rotating elements (the Kramers chain) as long as the number of elements is large, and it gives a *reasonable approximation* for the entropy of chains of finite length” (Kröger, 2004: 463).

Now, if we want to take the statistical analysis of this section over the possibility of distribution within the fluid of the polymer chain, we would arrive at the following distribution function $\psi(\mathbf{Q}, t)$:

$$\frac{\partial \psi}{\partial t} = \frac{2k_B T}{\zeta} \Delta \psi + \frac{2}{\zeta} \nabla \cdot \{\mathbf{F} \psi\} - \nabla \cdot \{(\kappa \cdot \mathbf{Q}) \psi\} \quad (11)$$

where T is the absolute temperature, k_B is the Boltzmann’s constant and $\mathbf{F} = \mathbf{F}^{(\text{FENE})}$. This model originally described a one-particle-distribution. Nonetheless, more elaborate versions have since been introduced, such as the FENE equation for dilute solutions where hydrodynamic interaction is involved. In this case, equation 11 would be generalised to:

$$\frac{\partial \psi}{\partial t} = \sum_{i=1}^N \frac{\partial}{\partial r_i} \left(\kappa r_i + \frac{1}{\zeta} \sum_j H_{ij} \cdot F_j \right) \psi + \frac{k_B T}{\zeta} \sum_{i,j} \frac{\partial}{\partial r_i} \cdot H_{ij} \cdot \frac{\partial}{\partial r_i} \psi \quad (12)$$

This is for the configurational distribution function $\psi(t, r_1, r_2, \dots, r_N)$ of a chain with N beads, taking into consideration that the Hydrodynamic Interaction (HI) matrix would be: $H_{ij} = H(r_{ij}) = \delta_{ij} + 1 + \zeta \Omega(r_{ij})$. As for the movement of the beads, it is described by a stochastic differential equation equivalent to equation 12:

$$dr_i = \left(\kappa r_i + \frac{1}{\zeta} \sum_j H_{ij} \cdot F_j \right) dt + \sqrt{\frac{2k_B T}{\zeta}} dS_i \quad (13)$$

where $dS_i = \sum_j B_{ij} \cdot dW_j(t)$, W denotes Gaussian white noise vector; B is related to the HI matrix through the fluctuation–dissipation theorem $H_{ij} = \sum B_{ik} \cdot B_{jk}^T$, and F_j denotes the sum of springs’ forces on bead j.

In fact, Kröger traces 16 variations of FENE model (Kröger, 2004: 458), such as FENE for Linear flexible classical polymers, FENE-n for branched flexible classical polymers and FENE-L, which is a second-order L-shaped closure model for FENE chains.

The important element in this model (models) is that for the model describing two beads or over, the calculations would be so difficult requiring computer computation to arrive at any result. In spite of that, equation 12 cannot be solved in closed form. There is a need to replace the random variable Ω_i by its equilibrium

average. Therefore, $H_{ij} = \delta_{ij} + h^*(1 - \delta_{ij})(2/|i - j|)^{1/2}$ where h^* is an HI parameter that is equal to:

$$h^* = \frac{\zeta}{6\pi\eta_s} \sqrt{\frac{H}{\pi k_B T}} \quad (14)$$

where H is the bead–spring coefficient and h^* , as well as the chain limits, can be experimentally and analytically determined.

In this case, the final outcome of such variation of FENE is not directly derivable from FENE; precisely because the h^* is an additional parameter determined empirically and is not part of FENE.

4. DISCUSSION

In sections 2 and 3, a very sketchy picture about modelling in polymers has been given. Although limited to models of liquid polymers, it was demonstrated that capturing the properties of such polymers was not possible within a single model. Even when using computer simulation methods “the broad range of timescales and underlying structure prohibits any one single simulation method from capturing all of these processes” (Glotzer et al., 2002: 401).

A starting point in any review of theoretical representation of polymeric structure would always remind the reader that polymers couldn’t be modelled by using a single model, but rather many models. One of these review papers had this to say in the introduction: “Polymeric structures in melts, blends and solutions can range from nanometre scales to microns, millimetres and larger. The corresponding time scales of the dynamic processes relevant for different material properties span an even wider range, from femtoseconds to milliseconds, or even seconds or hours in glassy materials or for large scale ordering processes such as phase separation in blends. No single model or simulation algorithm can span this range of length and time scales. Therefore, molecular and mesoscopic models for polymeric materials range from those including quantum effects and electronic degrees of freedom; to chemically realistic, classical models; to coarse-grained, particle-based mesoscale models that retain only the most essential elements of the polymer system to be simulated; to field-theoretic models that describe the polymer system in terms of density or composition variables” (Ibid: 401-402).

Such a long quotation is important to highlight the scale of the problem of modelling in polymers. As we can

see, models are “ranging” through different types of theoretical justifications of these models. In fact, these theoretical justifications are necessary only because models are looked at as partial representations “reflecting” the accepted theories of physics. This conceptualisation of models would alter dramatically if we reverse the priorities; that is, if we accept that models are developed as to represent phenomena, while theories used in crafting such models are mere tools, then we can understand the great variety of models at hand in polymers.

The story would not stop there; the most difficult task confronting polymer physicists is to synchronise these models and to get these models to correspond to each other at the boundaries. Moreover, they need to be able to show how the microscopic structures would in fact produce the macroscopic behaviour, not to mention the usual problems in this regard: who would decide on the boundaries? How can we be sure that such boundaries are the real separation in using this or that model? If nature is a continuum, why should we accept that these boundaries really exist? Why do we need more than one model to express the one and the same natural entity?

Of course some would say that the problems here are not important so long as all these models are derived or anticipated from the fundamental theories of physics, and therefore, if we can solve the basic problems in physics inherent in linking the micro and macro theories of fundamental physics, these sub-problems would be no more than exercises in mathematics. Hence, because we can correspond classical with quantum mechanics, for example, there is no problem in finding the lines linking these models stemming from the two theoretical approaches when applied to polymers.

This is what is hard to agree with. Primarily, because the real models that express the polymeric behaviour are not directly derivable from these fundamental theories. As was observed in the limited examples given earlier, these models need additional empirical parameters characteristic of the type and structure of the real polymer that is described by such models, at least in the case of the simple linear models described in section 2. As for the more complex non-Newtonian models in section 3, it was obvious that these models would use mathematical structures that are seemingly (by form only) similar. But these models would change the parameters, the rate, and the cross section of the chosen chain that would change in effect the number of beads in that section and the expected outcome behaviour of

the polymer structure, moreover, the number of approximations and further approximations that are used to arrive to the final model.

In each case, there will be some kind of negotiation between the theoretical expectation with the simulation resulting from it and the experimental verification for the studied polymer. In the course of the negotiation, the expected theoretical model would lend some relaxation of its frame to the experimental findings, and through this process, the value of the parameters would change. This change would result in changing the corresponding mathematical expression correlated with that parameter. As Kröger pointed out, in such situations caution is necessary in interpreting some of the results:

“Simulation has to deal with quantities in terms of reference units for mass, length and energy. These have to be obtained by comparing experiment with simulation and provide the basic length (σ) and energy (ϵ) scale of the LJ potential as well as the mass (m) of a bead in solving Newton’s equation” (Kröger, 2004: 485).

As we can see, the idea is to find a way of comparing experimental results with computer simulation in order to be able to trace back the possible mathematical formation that would reproduce through simulation acceptable results that would close (through approximation and experimental error) to the experimental results.

In effect, this process is dependent on results to trace back and change (improve) the theoretical conception used. As Gorban et al. (2003) tells us:

“Dynamic and static *post-processing procedures* give us the opportunity to estimate the accuracy of obtained approximations, and to improve this accuracy significantly” (Gorban et. al., 2003: 1).

They conclude from their review of models on polymers that do not tally with the mathematical vision of starting with the differential equation of a system, but rather depend on another way of theory building, as they put it:

“Final identification of the model is always done on the basis of comparison with the experiment and with a help of fitting. For this purpose, it is extremely important to reduce the dimension of the system, and to reduce the number of tunable parameters” (Ibid, P 207).

This is a clear expression of the way phenomenological models are built: from a bottom-up approach. The adaptation of the mathematical structure

will not stop at presenting the raw data, but rather this is only the starting point for a further process to take place. The mathematical structure needs further adaptation to be able to capture the corresponding limit between the level the model operates through and the other levels indicated by the arbitrary sections set by the accepted technique. It should be emphasized here that different theoretical techniques within polymers would disagree on the arbitrary sections. As for the techniques used to connect between the different levels of description, at least eight techniques are in operation, which might in a way correspond to the main clusters of models in polymers, to mention but some: Boltzmann equation, GENERIC equations, stress tensors, etc...

Moreover, modelling of one particular point would not be restricted to the use of one suggested model, but might have more than one “successful” model, such is the case for modelling fluids with microstructure. In this case Kröger tells us:

“There are various approaches in the literature to modelling fluids with microstructure.”

One of these approaches is the structural approach, which is based on averaging the trace of motion of individual particle in a Newtonian fluid. In addition, as usual, in order to be able to obtain a more “concentrated” system, various approximations to the particle motions have been used. Nevertheless, such a model is not the only one:

“Alternatively, ‘phenomenological’ continuum theories for anisotropic fluids have been postulated. They tend to be quite general, being based upon a small number of assumptions about invariance, perhaps the most successful and well-known example being the EL⁸ director theory for uniaxial nematic liquid crystals. Additionally, numerous models have been developed and discussed in terms of symmetric second- and higher-order tensorial measures of the alignment” (Kröger, 2004: 512).

At this point, the question of the author would, rightly, be: “if and how such diverse approaches may be interrelated?” These processes are looked at as phenomenological and are accepted as a common practise in modelling polymers, even though, under the influence of fundamentalism in science, this is not accepted as the final word. Let us take one example of such position:

“Although closed-form phenomenological models have been widely used in research and commercial

codes, their degree of success is limited because of a lack of physical ingredient on the molecular level” (Ibid: 461).

This is nearly echoed in another statement:

“The phenomenological description of the viscoelastic behaviour of amorphous polymers in the region where deviations of the SOR appear has been adjusted many times within the last decades” (Ibid: 483).

Another point can be drawn from modelling of polymers, as well as from modelling in applied physics; some of the words that are used in such processes would be puzzling for philosophers, such as the phrase “for convenience”. Such a phrase is used when physicists are not able, due to practical constraints or lack of theoretical understanding of the exact behaviour of the studied phenomenon. At such a point, physicists would use the phrase to overlook certain elements that would otherwise be difficult to incorporate into the used model.

Physicists would acknowledge the limitation of their models in dealing with real structures; in our case, Kröger would put it in the following way:

“Various experimental observations reveal an important aspect of the behaviour of polymer solutions which is not captured by FENE dumbbell models.”

But the author knows the importance of universality to the theories of physics, so he highlights the universality of the experimental behaviour rather than the universality of the FENE model:

“When the experimental data for high molecular weight systems is plotted in terms of appropriately normalized coordinates, the most noticeable feature is the exhibition of universal behaviour. By this it is meant that curves for different values of a parameter, such as the molecular weight, the temperature, or even for different types of monomers can be superposed onto a single curve.”

But he then admits that he is using “universal” in a rather special way:

“There is, however, an important point that must be noted. While polymers dissolved in both theta solvents and good solvents show universal behaviour, the universal behaviour is different in the two cases.”

If the case that we are dealing with two unrelated universals that are operating on a generic type of phenomenon, the previous comment will not have any effect. But what the author goes on to explain is what makes this remark astonishing:

An example of this is the observed scaling behaviour of various quantities with molecular weight. The scaling is

⁸ Ericksen-Leslie Theory.

universal within the context of a *particular type* of solvent. The term *universality class* is used to describe the set of *systems* that exhibit common universal behaviour. Thus theta and good solvents belong to *different universality classes*" (Ibid: 471) (my italics, T. S.).

The universal is here universal within a particular type, and to differentiate such "universal" from what is usually understood by it, the term "universality class" is introduced to mean a certain type of universality that is related to a "particular type", and that would lead to accept these two behaviours, that are part of the behaviour of liquid polymers, as belonging to two "different universality classes".

5. CONCLUSION

The case of modelling of polymers highlights the

importance of looking at theorisation in physics in a new way. It is not any more obvious what fundamentalists of theoretical physics are trying to sell us by assuring the importance of fundamental theories as the underlying base of any understanding of any physical phenomena. If such theories would not be able to help us in understanding these phenomena unless we accept what the theories state as boundary conditions, and after "purifying" the phenomena from any "outside" interaction, then, do we in fact understand the phenomena as such or we understand the exact parts these theories want us to see of the phenomena (or what these theories want us to believe to be the phenomena)? In applied physics, nature is who is in charge. Theories are important and essential in arriving at the specific models, but these models do not obey the theory conditions but rather conditions of nature.

REFERENCES

- Anderson, P. 1972. More is Different, *Science*, 177: 393-396.
- Cartwright, N. 1999. *The Dappled World*, CUP, Cambridge.
- Cartwright, N., Shomar, T. and Suárez, M. 1995. The Tool Box of Science, in *Poznan Studies in the Philosophy of the Sciences and the Humanities, Theories and Models in Scientific Processes*, W. Herfel et al. (eds.), 44, Rodopi, Amsterdam.
- Doi, M. and Edwards, S. 1986. *The Theory of Polymer Dynamics*, Clarendon Press, Oxford.
- Glotzer, S. and Paul, W. 2002. Molecular and Mesoscale Simulation Methods for Polymer Materials, *Annu. Rev. Mater. Res.*, 32: 401.
- Goldenfeld, N. and Kadanoff, L. P. 1999. Simple Lessons from Complexity, *Science*, 284: 87-89.
- Gorban, A., Karlin, I., Ilg, P. and Öttinger, H. 2001. Corrections and Enhancements of Quasi-equilibrium States, *J. Non-Newtonian Fluid Mech.*, 96: 206.
- Gorban, A., Karlin, I. and Zinovyev, A. 2003. Constructive Methods of Invariant Manifolds for Kinetic Problems, Preprint, the www, p1: http://owl.ethz.ch/d-werk/oettinger/MK_DIR/pag9/paper.pdf.
- Halin, P., Lielens, G., Keunings, R. and Legat, V. 1998. The Lagrangian Particle Method for Macroscopic and Micro-Macro Viscoelastic Flow Computations, *J. Non-Newtonian Fluid Mech.*, 79:387-403.
- Kröger, M. 2004. Simple Models for Complex Nonequilibrium Fluids, *Physics Reports*, 390: 453-551.
- Laudan, L. 1981. A Confutation in Convergent Realism, *Philosophy of Science*, 48: 19-49.
- Laudan, L. 1984. Explaining the Success of Science, in J. Cushing (ed), *Science and Reality*, Notre Dame University Press, Notre Dame.
- Lozinski, A. and Chauvière, C. A fast Solver for Fokker-Planck Equation Applied to Viscoelastic Flows Calculations, Preprint, the www: <http://www.dam.brown.edu/scicomp/publications/Reports/Y2003/Brown-SC-2003-01.pdf>.
- Morrison, M. 1997. Mediating Models: Between Physics and Physical World, *Philosophia Naturalis*, 34.
- Morrison, M. and Morgan, M. (eds). 1999. *Models as Mediators*, CUP, Cambridge.
- Shomar, T. 2000. Realism with a New Face, *University of Tabriz*, Tabriz.
- Shomar, T. 1999. *Phenomenological Realism, Superconductivity and Quantum Mechanics*, PhD, London School of Economics, London.
- Strobl, G. R. 1997. *The Physics of Polymers*, 2nd Ed., Springer, New York.
- Van Fraassen, B. 1980. *The Scientific Image*, Clarendon Press, Oxford.
- Van Fraassen, B. 1985. Empiricism in the Philosophy of Science, in P. Churchland and C. Hooker (eds), *Images of Science*, University of Chicago Press, Chicago.
- Warner, H. R. 1972. Kinetic Theory and Theology of Dilute Suspensions of Finitely Extensible Dumbbells, *Ind. Eng. Chem. Fundam.*, 11: 379-387.

:

*

(CPNSS)

.2006/5/9

2005/9/11

*
