So, Who's Afraid of Nonlinear Regression?

Heinz Plaumann, Ph.D.
BASF Corporation, 1609 Biddle Ave., Wyandotte, MI 48192, USA

ABSTRACT

Many technical and business colleagues shy away from maximizing the true value of decision-supporting data due to reluctance to analyze data with the most up-to-date, descriptive and predictive models. Sometimes, this entails the development and fitting of nonlinear models.

This paper presents several examples from industry. The first uses SAS-JMP software to fit models derived to support our work in product development improving performance of professional level bowling balls. This was coupled with extensive use of experimental design and led us to strong structure-property relationships, including the "subjective" evaluation of the end product: Is this really a better bowling ball?

A second example involves developing understanding in a spray application in agriculture where we applied models to rheological behavior and spray particle size distribution.

Final examples involve analysis of market penetration data. A modified Fisher-Pry model was used to show that our timing in development and market introduction was "just right" for a new family of products for use in automobile interiors. It also helped guide decisions in several cleaning areas.

Introduction

The reduction of data to descriptive or predictive models is often a laudable goal in business. We frequently review market data, invest heavily in R&D, pore over sales and production data hoping to identify trends to make us "smarter": What really happened in these product development experiments? Where do we think this new development will fit best? Where is the market going? Will we be there with the right product at the right time? Such data from diverse sources and of diverse nature help tremendously in this regard…if we can only understand the relationships among them.

The use of models linear in their parameters (hence using linear regression) is widely used, especially with the advent of user-friendly spreadsheet programs on almost everyone's desktop computer or laptop (many programmable calculators too!). However, the world is not as linear as we may wish it to be, frequently being best described with exponential, logarithmic or more complex relationships. We frequently invoke all manner of linearization methods to “straighten the world out” so that we can use the user-friendly tools readily available to us. This may allow us to understand relationships and correlations more easily. However, we may distort such features hidden in the data as error structure, leads us to believing another mechanism is operative or limit the quality of our forecasts. These drawbacks can be overcome by using the “true” or “best” model we know or can derive for analyzing the data and performing forecasts. Many such models have direct phenomenological implications as rate equations for growth or chemical processes.

SAS-JMP software has available a very easy-to-use nonlinear regression option, no more complex that its normal regression or data analysis tools (1). We describe here two cases where we used the true power of this feature, in one case to analyze data to lead to improved product development and in the other to forecast growth and movement in a new market for our business.

Nonlinear Regressions

There are many algorithms for nonlinear regressions, most of which depend upon some steepest descent methods to minimize the sum of squares of the residuals after fitting is completed. Some, such as the simplex method, are best described geometrically. Many other methods exist. Nonetheless, the use of such methods does not appear to be as widespread as we wish among either technical or business colleagues, I can only assume because the tools are not as readily available or as easy to use as we believe.

Case I: Designing a Better Bowling Ball

The performance of a bowling ball is best described by two performance factors: So-called “hook”, the ability of the ball to curve into the pins to maximize the number of pins knocked down, and the ability to maintain this hook as the ball is used repeatedly. Professional-level bowling balls typically cost of the order of \$300 - \$1000, are used for up to 300 games, then “lose their hook”. They often have multi-layer structures with an external coverstock, a core concentric to the coverstock and sometimes an additional weighted core of specially designed geometry, all intending to optimize hook performance as the bowler applies the laws of momentum and inertia through spin and speed to the ball.

We undertook a significant product development activity several years ago, to improve both the hook behavior and its consistency. (See references 2, 3). As part of this, we studied the uptake of the coverstock material of mineral oil used to lubricate the bowling lane. This was investigated by casting small plaques of polymer and immersing them into the oil and monitoring their weight change. A simple mass transfer model for a solid slab has this typical form (4):

$$E(t) = E_a E_b E_c = \left(\frac{8}{\pi^2}\right)^3 \exp\left[\frac{-D\pi^2 t}{4}\left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}\right)\right]$$

Since the coupons varied negligibly in geometry, parameter consolidation yields this reduced form:

$$E(t) = k \exp\left[- \theta t \right]$$

Our initial observations showed that the coupons first gained in weight (eureka!) and decreased in weight to an asymptotic value. Related characterization of the polymer surface by atomic force microscopy (AFM) revealed a distinct roughness or porosity in some of the samples. Through problem solving discussions, we arrived at a model in which the oil filled surface and near-surface voids initially (a fast process) and then underwent diffusional exchange with a plasticizer used in the formulation (higher density than the lubricating oil). We arrived at this final model for this process:

$$M(t) = m_i \left[\exp\left(- \theta_p t \right) \right] + m_{fo} \left[1 - \exp\left(- \theta_{po} t \right) \right] + m_p \left[\exp\left(- \theta_p t \right) - \exp\left(- \theta_{po} t \right) \right]$$

.

The model has a term for each of the processes: Void filling, exchange of liquids of different densities, and an interaction product.

The SAS-JMP software's nonlinear regression option was used in fitting this model (Figure 1). We had considerable difficulty in reaching convergence and elected to secure initial parameter estimates by separating the effects of each process: Placing a coupon in plasticizer until steady-state was achieved, or until "void-filling" was complete, establishing the rate constant for this process, removing the coupon to immersion in oil. For several samples, we repeated this cycle several time (observing complete reversibility, no hysteresis). Using these initial parameter values did not provide convergence in the full model above. Perhaps invocation of a more sophisticated parameter estimation method (5) would have proven useful. Nonetheless, we had sufficient information to proceed in our product development.

This information, although seeming only academic in value, allowed us to screen coverstock materials quickly knowing that non-porous or too porous materials would not deliver the desired hook and retention of the hook.

Case II: Spraying Agricultural Chemicals

Many agricultural chemicals are applied in either granular or spray form. Control of the spray process can be critical to the effectiveness, preventing overspray and loss of active ingredients due to wind drift (6). We have attempted to develop relationships among fundamental chemistry, flow behavior (rheology) and spray behavior. These are highly nonlinear systems, giving such behavior given in Figures and . Polymer melt systems deviating from simple Newtonian- behavior are often modeled adequately with such models as Power Law (7) or Carreau (7) models. These posed great difficulties for us in term of fitting and achieving convergence (reasons to be learned later!). We then developed our own DIY Power Law derivatives which worked adequately but we encountered some inconsistencies: As we increased the temperature, the fitted data deviated significantly from observed (Figures 2,3). Any model that does not fit should make us re-examine our assumptions and we concluded that we may be dealing with phase changes for the formation of microstructures in solution.

Additionally, control of wind drift is often attributed to reduction of the finest particles during the spray process. To develop these correlations, we also fitted log-normal distributions to the particle size observations (Fig. 4), attempting to create structure-property-performance correlations, much as in Case I above (8). We have not yet been so successful in this Case!

Case III: Forecasting Growth of New Technology

Technological change has accelerated over the past decades (9). The common adage "The computer you buy today is already out of date", underscores this. Business management guru Peter Drucker has expressed this rather dim view that "forecasting is not a respectable human activity and not worthwhile beyond the shortest periods" (18). Nonetheless, we can still examine the product life cycle (10) (Figure 5) and extract useful information. One model which is appropriate to describe the early stages of the substitution process, in which a new technology replaces an old, up to the "plateau" is the Fisher-Pry model (11, 12):

$$f = 0.5 \left\{ 1 + \left[\tanh \quad a\,(t - t_0) \right] \right\}$$

where:

f = fraction of new technology penetration into market
a = rate constant for substitution process
t = time (year)
t_0 = "half life" of substitution process

Models such as these can prove useful in developing business cases for strategic acquisition or R&D investment, developing marketing strategies for products in their various growth phases, or ensuring the logistics or supplies issues are resolved. The half-life is not only significant as the point at which the substitution is half complete. It is also the point of inflection, the time point at which the growth occurs the fastest!

We used the Fisher-Pry model to examine the potential growth of polyurethane materials replacing other materials in construction of instrument panel skins, surfaces having a nice comfortable leather-like feel (13). We secured market share data representing the growth of the new technology (14). The model suffers a few weaknesses:

1. From its mathematical form it asymptotically approaches zero but there is indeed a time at which there were, for example, no electric light bulbs replacing candles. That is, there truly is a time when market share = 0.
2. It assumes that the replacement approaches 100%. In many cases, the substitution may be nearly complete (one can still buy buggy whips but they are harder to find!). Oftentimes, the substitution stops earlier with market saturation or the advent of an even newer technology driving the "new" one into decline.
3. Generally, one can only secure one market share data point per time unit, often times, one per year. For rapid substitutions, the future will be upon us before we can forecast it!
4. As the data are not experimental observations, we have no replications or way to estimate error.
5. All of the early data will obviously be to the left of the point of greatest growth rate, t_0. It is often expedient to have data covering the entire range effecting the modeling process.

A simple variant of the Fisher-Pry model for the "regressive weak at heart" is the linearized version. However, with the power of SAS-JMP software at our fingertips, we used the model as above with the only six market share data available. We obtained an estimate of t_0 = 2011, a plausible time for the new technology to have replace half of the competing technologies. (Figure 6). Since we find it likely that new technology will not fully replace the incumbent competing ones, we modified the Fisher-Pry model by multiplying it bu the new parameter f_{max}, the market share at the maximum substitution of the old technologies.

Several others examples where we have found use of the Fisher-Pry model of benefit include replacement of household top-loading laundry machines by front-loading (17)(Fig. 7). A particularly challenging analysis examined trends in the dishwashing detergent market in North America where it appears powders are in decline but other forms such are gels or single-dose packs are growing. The point of particular interest here is that, for consistency in parameter estimation, the Fisher-Pry model should be applied to all three sets of data simultaneously, constrained by the fact that the sum of the market shares equals 100% (Fig. 8). Any way one looks at it, it is certainly an easy way to have a discussion/near-argument at any office coffee machine discussing this topic!

Just for fun, in learning about use of the Fisher-Pry model, we also examined a few societal trends: Proportion of U.S. homes having home computers (16) and internet access (16). The model appeared to work well, with one alarming point: It appears that more than 96% of U.S. homes will have computers by about 2020, however internet access may taper off at about 70%.(Figures 9, 10). This should set our network providers and sociologists to work, analyzing reasons for this! Of course, additional data points for the next few years could greatly sway this forecast!

Conclusions and Suggestions to improve SAS-JMP Software:

We have applied the user-friendly SAS-JMP software's nonlinear regression capabilities to help us in product development, business planning and forecasting. The information thus gleaned has helped us make more intelligent decisions leading to improved commercial success.

It would be of advantage also, if the software could provide additional information about the parameter estimates, a covariance matrix for example. Even better, pair-wise confidence contours for the parameter estimates would be of great value.

Otherwise, it's just a very nice program. Thanks SAS!

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14. Provided by Eller and Associates and by Market Search, Inc.
15. J. Martino, “Technological Forecasting for Decision Making, Second Edition”, North Holland Press, 1983, p.66.
16. U.S. Census Bureau Report “Computer and Internet Use in the United States: 2003”, issued 2005

17. Market data provided by Information Resources, Inc., Chicago, IL.
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Figure 1: Oil Uptake in Bowling Ball Coverstock Coupons

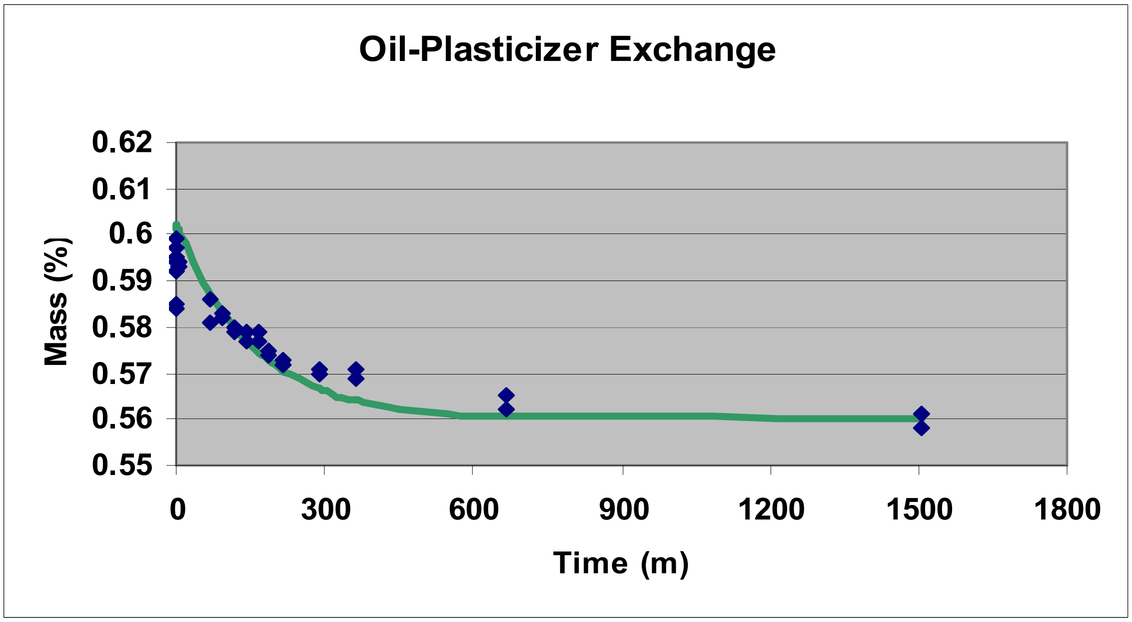


Figure 2: Viscosity of Thickener in Water Solution at 25C (Series 1, 2 Replicate Observations. Series 3 Model)

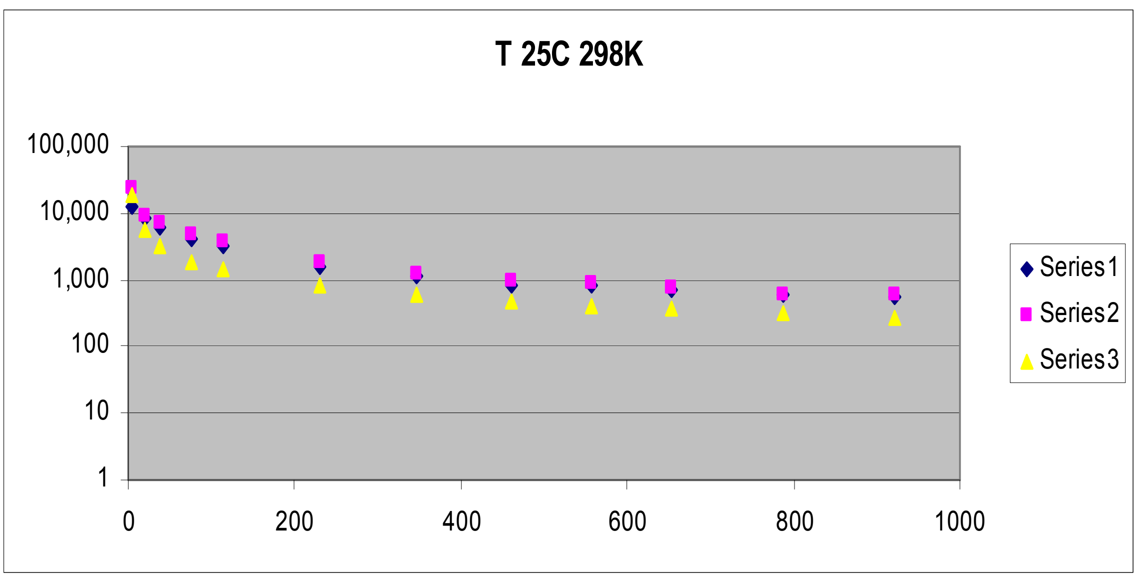


Figure 3: Viscosity of Thickener in Water Solution at 55C (Series 1 model, Series 2 observed)

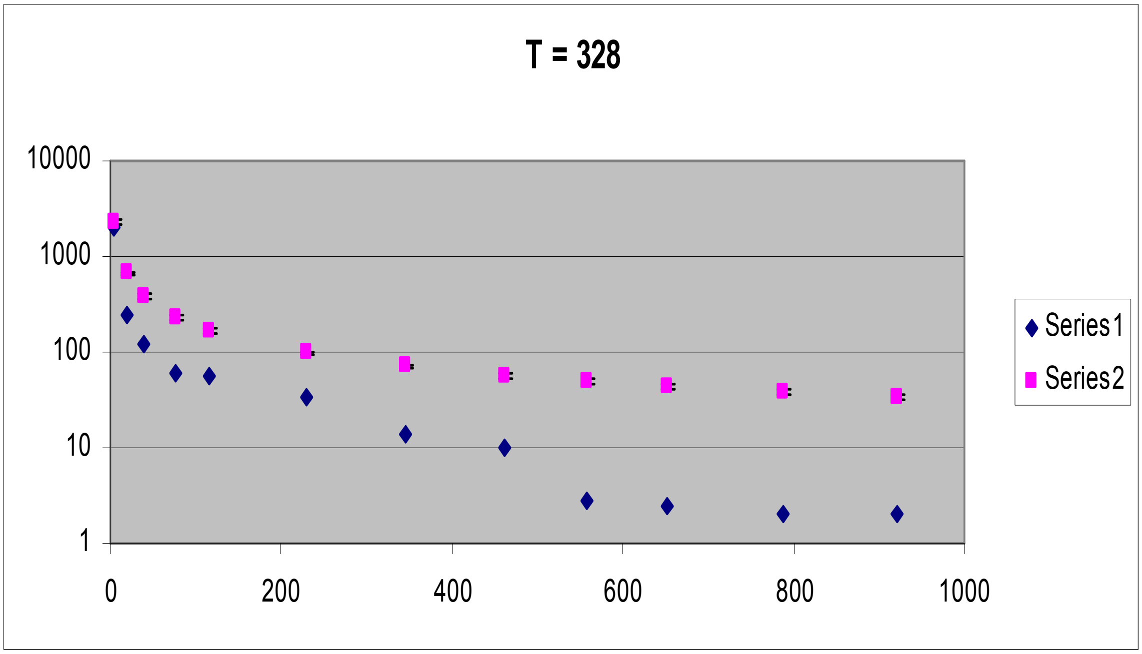
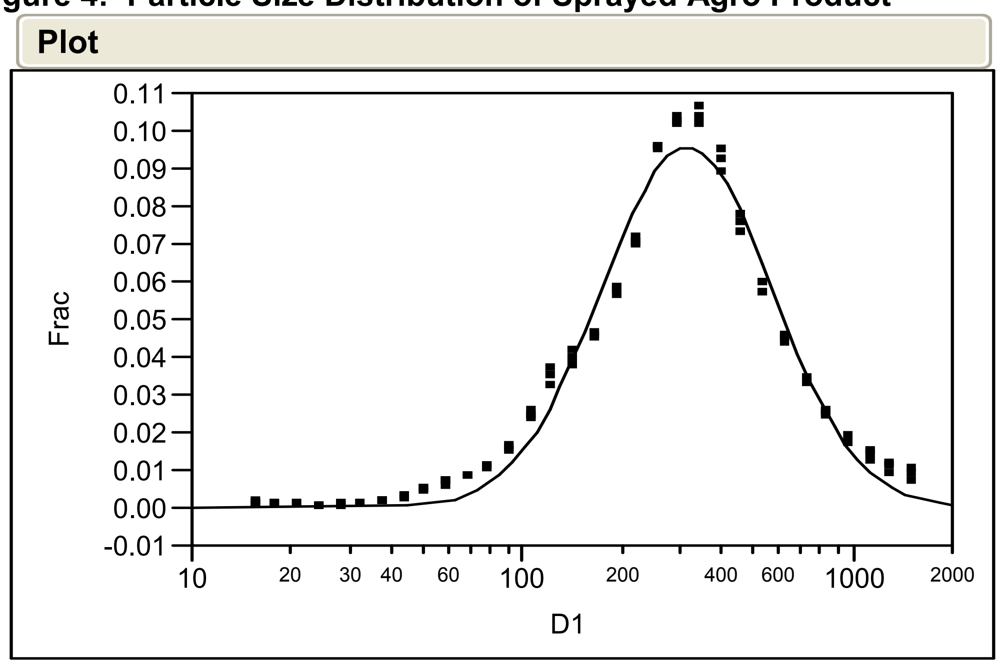


Figure 4: Particle Size Distribution of Sprayed Agro Product



Parameter	Estimate	Low	High
dbar	314.15868098	6.84e-6	0.00002
s	0.5941082034	7.63216	22.8965
a	0.0957199115	-0.1079	-0.036

Figure 5: Product Life Cycle

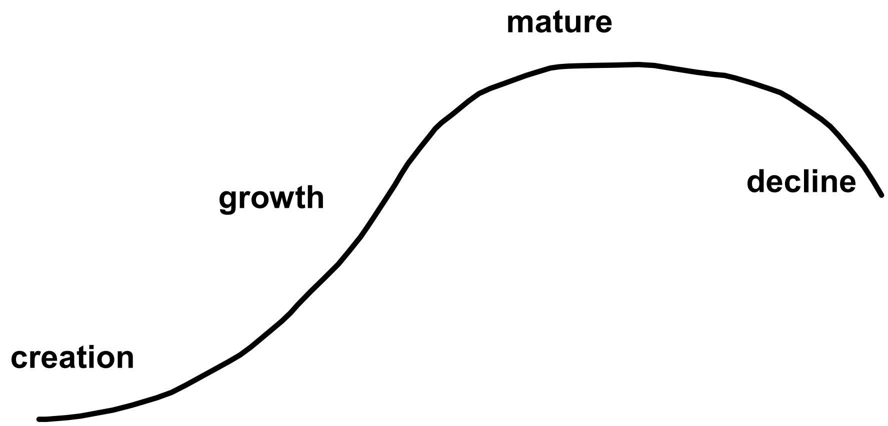


Figure 6: Fisher-Pry Model: Replacement of Other Instrument Panel Materials with Polyurethane Skin

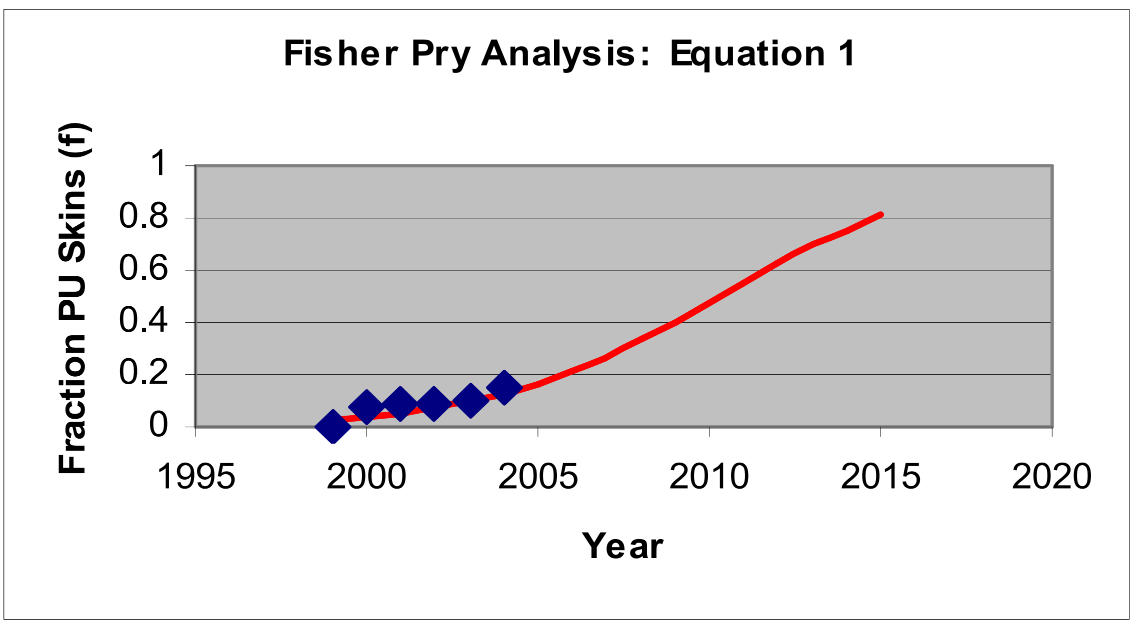


Figure 7: Market substitution of Top-Loading Washing Machines by Front-Loading Washing Machines.

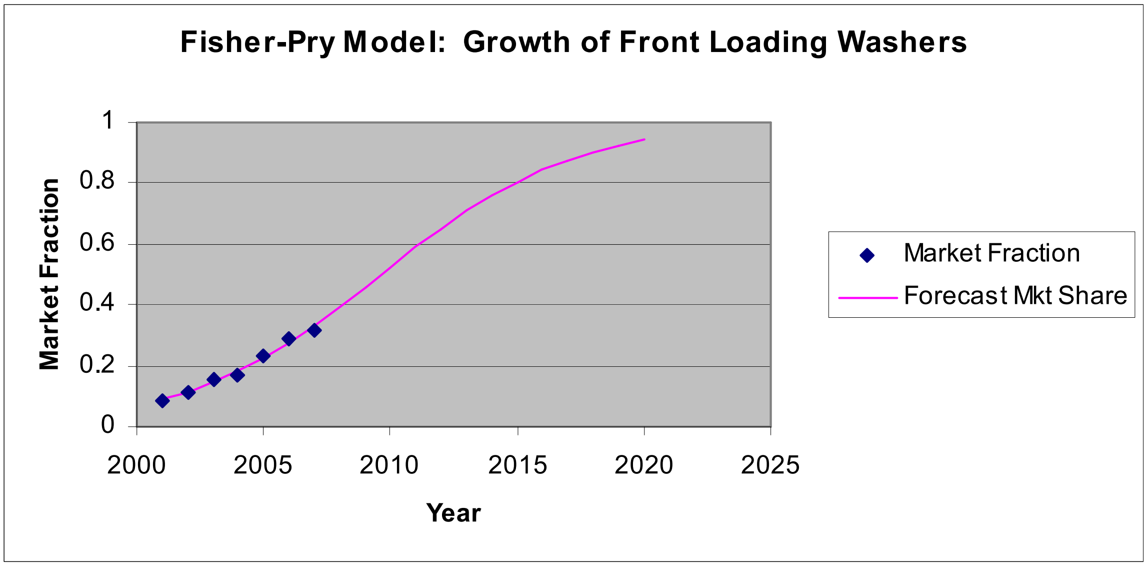


Figure 8: Dishwashing Detergent Trends in the North American Market

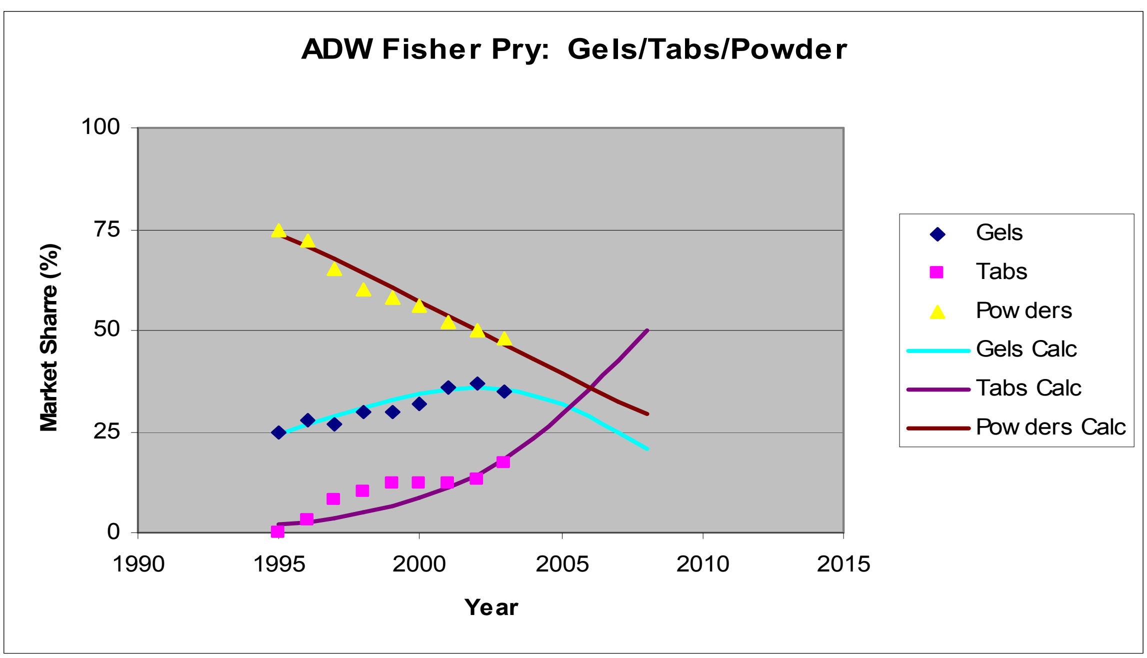


Figure 9: Fraction of U.S. Homes with Personal Computers

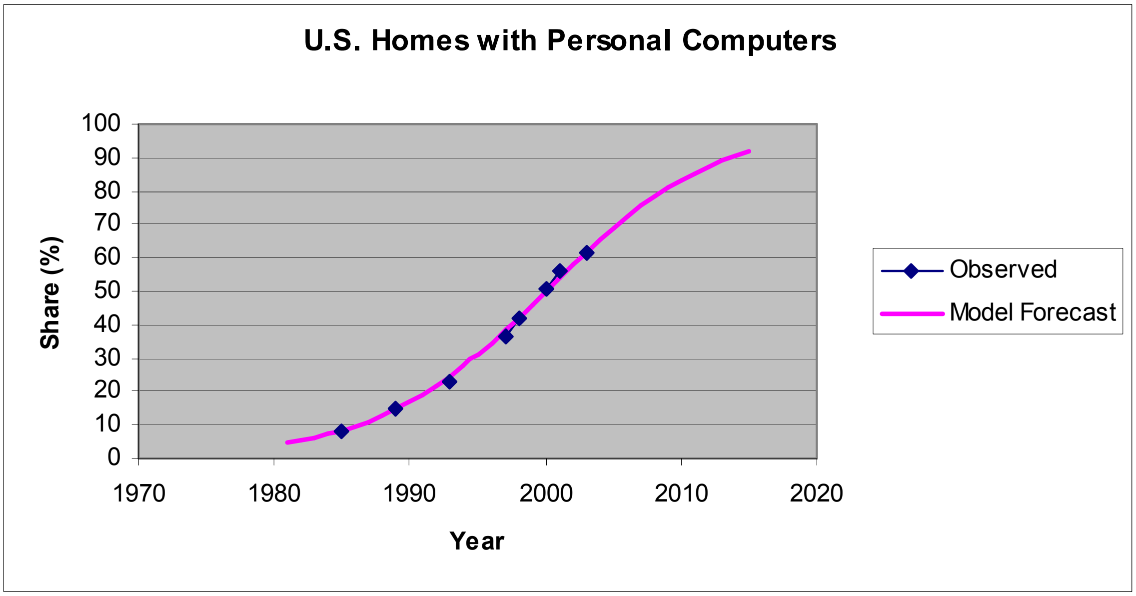
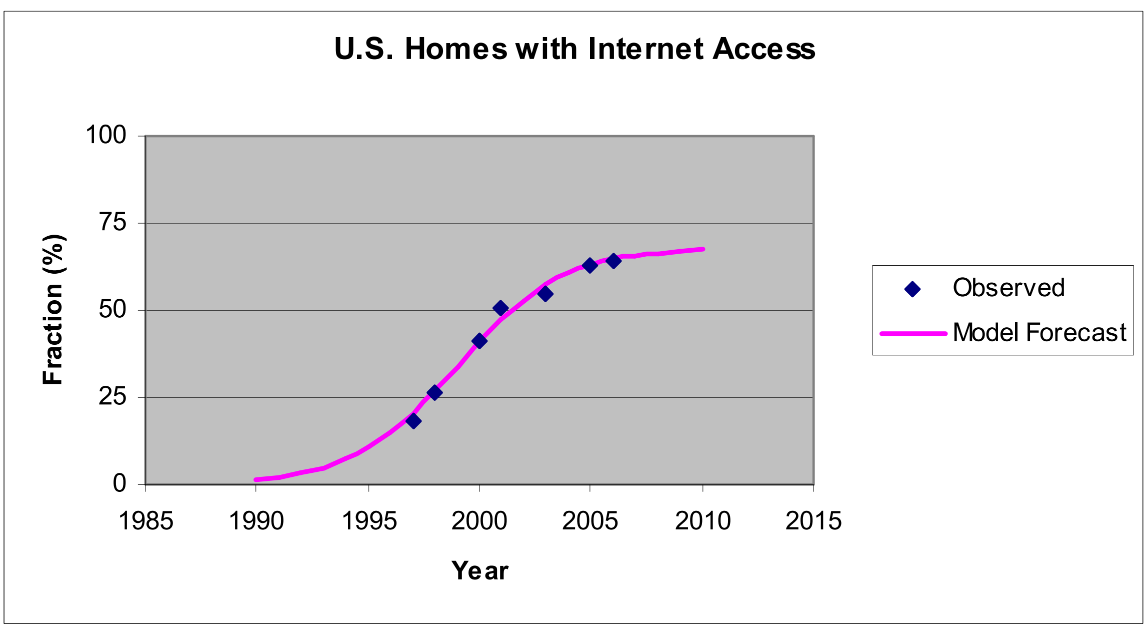


Figure 10: Fraction of U.S. Home with Internet Access



Heinz Plaumann, Ph.D.

- **University of Waterloo, Canada, Ph.D. Chemistry, M.A.Sc. Chem. Eng.**
- **Polysar Limited, 9 years, Synthetic rubber, Thermoplastic Elastomers, Composites, R&D/Production, Sarnia/Canada**
- **BASF Group:**
  - **10 years Emulsion Polymers, R&D/Marketing, Sarnia/Canada, Ludwigshafen/Germany, Charlotte/NC**
  - **7 years Urethanes, R&D, Schwarzheide/Germany, Wyandotte MI**
  - **2006 – Present, BASF Care/Performance Chemicals, R&D Wyandotte MI**
- **Experiences/Expertise: Broad range of polymer chemistries, syntheses, applications. Applied statistics. R&D/Technical Management. Hold ca. 20 patents, ca. 25 publications/presentations. College instructor, seminar leader.**
- **Hobbies: Recreational hockey, basketball, aerobic training. Square dancing. Jazz guitar/bass.**