

Predict the miscibility behavior of solvent and polymer systems

Identify regions of stability in bulk manufacturing processes

Predict the thermodynamics of mixing from the chemical structures of binary mixtures

## Blends

Blends is used to predict the miscibility behaviour of solvent and polymer systems and to give a good indication of the stability of these systems in bulk manufacturing processes. This is a simulation technique which predicts the thermodynamics of mixing from the chemical structures of binary mixtures, producing phase diagrams which identify regions of stability. Blends is a screening tool which enables the development of stable formulations, while reducing the need for laboratory experimentation using 'live' chemicals.

### Blends Applications

The miscibility of polymer and solvent systems is very important in many polymer processing operations such as for the preparation of adhesives, pharmaceuticals, cosmetics, and speciality surface coatings for metals, glasses, and plastics. Generally this type of formulation work will require considerable experimentation to develop the most cost effective formulations with highest possible polymer to solvent ratios. Formulation scientists will also be interested in developing stable base formulations then for example testing the effects of coalescing agents, pigmentation and dispersants, plus physical changes such as freeze-thaw cycles.



*The chemicals industry uses a wide range of organic solvents for its separation processes*

Formulators will be most concerned with phase separation which might either restrict the shelf life of their product or render it unusable.

Mixed solvent systems are used in many fine chemicals processes such as for solvent extraction, recrystallization and azeotropic separations. In these situations it is often desirable to select solvents with lowest cost and ease of recycling while influencing a phase change to occur within a very specific temperature range. Once a process has been implemented it is often very difficult to change the composition of the mixture without considerable investment in time and plant modifications.

Mixed polymer systems are particularly important in the preparation of composite materials for the transport and construction industry. Often the choice of polymer will be determined by balance of cost and mechanical properties of the composite material. The formulator will be interested to improve the compatibility of polymers with other materials outside of their normal service temperature and humidity range, e.g. for products for shipment to unusually hot or humid climates. Poor formulations might have very restricted geographical markets or shelf lives.



*Formulators of thermoplastics aim for optimal mechanical properties by blending pure polymers and additives*

### Blends offers:

- Faster product development and shorter time to market for new and improved formulations
- Reduced risk of product failure due to phase separation or ageing on storage and transportation
- Possibilities for optimizing the use of expensive solvents in fine chemical processes
- Opportunity to investigate the stability of formulations outside their 'in service' application range. Also a means to optimize shelf life.

### Features and Capabilities

- A practitioners tool for technicians, engineers, and formulation chemists
- Provides cost saving solutions for new product and process development
- Uses office desktop IT equipment, reduces the need for experimentation using 'live' chemicals in wet chemical laboratories and polymer processing equipment
- Versatile software package, applicable to many separate chemical components for incorporation in binary mixtures
- Fast turnaround several projects can be processed simultaneously
- Potential to use Blends alongside process engineering software for simulation of physical separations such as for solvent extraction, or azeotropic distillation
- Library facilities for storing pairwise molecular interactions.

### References

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Laboratory formulation studies often require extensive solubility and compatibility studies

### The Materials Studio Advantage

Blends is available through MS Modeling, Material Studio's modeling and simulation suite, that runs as a Windows® client on your PC, and provides a comprehensive range of software tools. Flexible client/server computing harnesses the power of a range of server technologies, to access leading methods in computational chemistry and materials science, delivering results direct to your desktop.

The introduction of Blends into the Materials Studio toolkit provides a specialist tool for the engineer, polymer scientist, or formulator with a rapid, easy-to-use approach to screening mixtures of polymers and solvents for use in base formulations and process development investigations.