Wolfgang Kaiser
Willy Schlachter

# Energy in Plastics Technology

## Theory and Practice



$\vartheta_{G1}=30\,°C$   $\dot{m}_G$

$\dot{Q}_{VZ}$

$P_{elHZ}$

$\dot{m}_G=2.2755\ g/s$

$\vartheta_S=210\,°C$

$\dot{W}_A$

$\dot{Q}_{VW}$

200 °C    195 °C    190 °C    185 °C    180 °C

5 Barrel heating zones

Kaiser/Schlachter
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# The Authors

**Professor Dr. phil. Wolfgang Kaiser**

Wolfgang Kaiser studied chemistry at the University of Zurich. During his doctoral studies, he worked in parallel as a full-time assistant at the organic chemistry institute there from 1960 to 1962. In 1963, he received his doctorate (Dr. phil. nat). This was followed by several years of industrial activity in R&D in the field of additives (J.R. Geigy AG, Basel), and then the appointment as a professor at the University of Applied Sciences Northwestern Switzerland (formerly HTL Brugg-Windisch).

Decades ago, the author formulated the "theorem of plastics technology" for his students:

**Polymer raw material(s) + Additive(s) → Plastic**

This still facilitates access to plastics as a class of materials with its laws for many engineers.

On the occasion of his 70th birthday, Wolfgang Kaiser was awarded the Staudinger-Durrer Medal by ETH Zurich in recognition of his great achievements in the field of polymer materials. As "plastics emperor", he influenced hundreds of engineers in Windisch, and in later years also at the Department of Materials Science at ETH Zurich. In addition, he took over the establishment and operation of the Plastics Training and Technology Center (KATZ) in Aarau "extra-occupationally" and was its first managing director for many years. He is the founder of systematic education and training in plastics technology for engineers in Switzerland.

Wolfgang Kaiser is also the author and co-author of numerous scientific publications for engineers in the field of plastics technology.

**Professor Dr. sc. techn. Willy Schlachter**

Willy Schlachter studied mechanical engineering at the Swiss Federal Institute of Technology (ETH) in Zurich and obtained his doctorate at the Institute for Thermal Turbomachinery under Prof. Dr. Walter Traupel. He then worked at the Naval Postgraduate School in Monterey/California as a visiting assistant professor in teaching and research.

He began his industrial career as a development engineer at Brown Boveri-Sulzer Turbomaschinen AG. His further stations were: Head of Gas Turbine Development at Sulzer in Winterthur, Head of Department in the Thermal Machines Laboratory at BBC Brown Boveri in Baden, Mandate Technology in the Power Plant Division of BBC, and after the merger with ASEA at ABB.

He received a call to become a professor of Thermal Fluid Machinery at the University of Stuttgart, a position he could not accept for family reasons. He was appointed as a lecturer for mechanical engineering subjects and head of the mechanical engineering department at the then HTL Brugg-Windisch. He was vice-director and later director of technology at the University of Applied Sciences Aargau. His teaching activities were in thermodynamics, fluid mechanics, heat transfer, and power engineering as well as supervision of study and research projects in these fields. After the merger to form the University of Applied Sciences Northwestern Switzerland, he led the development of interdisciplinary research.

Willy Schlachter was co-author of a thermodynamics textbook and co-editor of the two volumes "Engineers Build Switzerland", published by NZZ Libro.

# Preface

The concept of "Energy in Plastics Technology" dates from the book "Energie in der Kunststofftechnik", published in German in 2019. The unforeseeable topicality that the subject of energy has experienced since that time was reason enough to revise the content of the present work and, where necessary, to adapt it to current circumstances. The fundamentals of the viscoelastic behavior of plastics in the solid state have been expanded. It goes without saying that the authors' primary aim has remained the same: to offer readers interested in technical and scientific matters a factually sound book as a guide to this interdisciplinary subject. The only exception is Chapter 10 (Recycling of Plastics), which cannot be treated independently of political will and social implementation.

For the didactic and methodological structure of the book, the previous successful three-part structure was deliberately retained. The focus is on a careful introduction to this fascinating field.

The first part, comprising Chapters 1–5, contains introductory fundamentals as taught in bachelor courses in process engineering, mechanical engineering, or materials science. Where considered helpful, exemplary basic examples solved according to a uniform methodology are included at the end of the chapters for better understanding.

The second part, Chapters 6–10, deals with extended fundamentals, the explanations of which are often of limited value without additional theoretical knowledge, e.g. at master's level. In the same way as in the first part, solved examples of more complex problems are given at the end of the individual chapters.

An attempt has been made to convey the necessary basics for an introduction to this interdisciplinary field in a concise form. However, depending on the level of previous education, it cannot be ruled out that it may be necessary to consult textbooks on individual subject areas given in the bibliography.

The special field of mass transfer, which is closely related to heat transfer, is therefore limited to a description of air drying under atmospheric conditions. In addition, for reasons of space, an exact description of the fundamentals of electrical engineering is omitted.

In the concluding third part, Chapter 11, the practical aspects are discussed in detail. On broadly defined, i.e. interdisciplinary, problems, the methodical approach to the practical examples treated remains the royal road here as well. These are based on the author's own experiments and those of others, as well as on the collection of data from renowned planners, leading machine manufacturers, and globally active companies in the field of plastics processing.

Last but not least, this book sees itself as a link between helpful theory and urgently sought solutions to problems in practice. In this way, it also attempts to facilitate access to theoretically more demanding textbooks and publications.

May the book be useful to the reader in learning, teaching, reference, and as a guide.

Wolfgang Kaiser and Willy Schlachter, July 2023

# Contents

# List of Symbols

## ■ Greek Characters

| Symbol | Description | Unit |
|---|---|---|
| $\alpha$ | Coefficient of heat transfer | W/(m$^2$·K) |
| | Absorptivity, subscript λ: spectral absorptivity | – |
| | Linear thermal expansion coefficient | K$^{-1}$ |
| $\beta_V$ | Spatial thermal expansion coefficient | K$^{-1}$ |
| $\beta$ | Radius ratio, Equation 9.71 | – |
| $\beta$ | Coefficient of mass transfer, subscript m: mean value | m/s |
| $\dot{\gamma}$ | Shear rate, subscript rep: representative shear rate, Figure 9.8 | s$^{-1}$ |
| $\Delta$ | Symbol for difference | – |
| $\Delta G_R$ | Free reaction enthalpy | J/kg, kJ/kg |
| $\Delta G_{Rm}$ | Molar free reaction enthalpy | J/kmol, kJ/kmol |
| $\Delta H_A$ | Activation enthalpy | J/kmol |
| $\Delta H_R$ | Reaction enthalpy (also enthalpy of reaction) | J/kg, kJ/kg |
| $\Delta H_{Rm}$ | Molar reaction enthalpy | J/kmol, kJ/kmol |
| $\Delta S_R$ | Reaction entropy (also entropy of reaction) | J/(kg·K), kJ/(kg·K) |
| $\Delta S_{Rm}$ | Molar reaction entropy | J/(kmol·K), kJ/(kmol·K) |
| $\delta$ | Flow boundary layer thickness, subscript T or $\vartheta$: thermal boundary layer thickness, subscript C: | m |
| | concentration boundary layer thickness | m |
| | Thin layer, Section 7.2 | |
| $\varepsilon$ | Emissivity, subscript λ: spectral emissivity | – |
| | Energy utilization | – |
| | Strain | – |
| $\varepsilon_{ij}$ | Coefficient of radiative exchange | – |
| $\varepsilon_R$ | Fin effectiveness | – |
| $\dot{\varepsilon}$ | Elongation rate | s$^{-1}$ |
| $\zeta$ | (Pressure-)Loss coefficient | – |

| Symbol | Description | Unit |
|---|---|---|
| $\eta$ | Dynamic (shear-)viscosity | Pa·s |
| $\eta$ | Efficiency | – |
| $\eta_C$ | Carnot efficiency | – |
| $\eta_R$ | Fin efficiency | – |
| $\eta_D$ | Elongational viscosity | Pa·s |
| $\theta(x, t), \vartheta(t)$ | Dimensionless temperature function | – |
| $\vartheta$ | Celsius temperature | °C |
| $\Delta\vartheta$ | Temperature difference | K |
| $\Delta\vartheta_m$ | Logarithmic mean temperature difference | K |
| $\vartheta_K$ | (Interfacial) Contact temperature | K, °C |
|  | Cooling limit: wet-bulb temperature | K, °C |
|  | Adiabatic saturation temperature, Section 8.3.2 | K, °C |
| $\kappa$ | Ratio of specific heat capacities $c_p/c_v$ | – |
|  | Isentropic exponent (ideal gas) | – |
| $\kappa$ | Annular radius ratio, Equation 9.68 | – |
| $\kappa$ | Compressibility, Equation 2.10 | $Pa^{-1}$ |
| $\Lambda$ | Dimensionless parameter, Equations 9.76 and 9.77 | – |
|  | Temperature wavelength, Figure 7.9 | m |
| $\lambda$ | Thermal heat conductivity | W/(m·K) |
|  | Friction factor (Darcy) | – |
|  | Wavelength (radiation) | m, µm |
| $\mu$ | Eigenvalue, Chapter 7 | – |
| $\nu$ | Kinematic viscosity, $\nu = \eta/\rho$ | $m^2/s$ |
| $\nu$ | Frequency | $s^{-1}$ |
| $\xi$ | Stefan correction factor, Equation 8.45 | – |
|  | Dimensionless radius, Equation 9.68 | – |
| $\rho$ | Mass density | $kg/m^3$ |
| $\rho$ | Reflectivity, subscript λ: spectral reflectivity | – |
| $\sigma$ | Axial stress | $Pa = N/m^2$ |
| $\sigma = 5.67 \cdot 10^{-8}$ | Stefan-Boltzmann constant | $W/(m^2 \cdot K^4)$ |
| $\sigma_0$ | Specific sublimation enthalpy ($H_2O$ at 0 °C) | J/kg, kJ/kg |
| $\tau$ | Shear stress | $Pa = N/m^2$ |
|  | Time constant, characteristic time | s |
| $\tau$ | Transmissivity, subscript λ: spectral transmissivity | – |
| $\phi$ | Fluidity (power law, Equation 9.1) | $(Pa \cdot s)^{-1}$ (Newtonian fluids) |
|  |  | $Pa^{-m} \cdot s^{-1}$ (non-Newtonian fluids) |
| $\varphi$ | Relative humidity, Equation 8.8 | – or % |
|  | Quality factor, Section 3.1.1 | – |
| $\omega$ | Angular velocity | $s^{-1}$ |

# ■ Latin Characters

| Symbol | Description | Unit |
|---|---|---|
| $a = \dfrac{\lambda}{\rho \cdot c}$ | Thermal diffusivity, subscript rep: representative thermal diffusivity, Section 9.8 | $m^2/s$ |
| $a_T$ | Shift factor, Equation 9.5 | – |
| $A$ | Surface area | $m^2$ |
| $b$ | Thermal diffusivity, Equations 2.6 and 7.37 | $W \cdot s^{1/2}/(m^2 \cdot K)$ |
| $b$ | Temperature coefficient, Equation 9.5 | $K^{-1}$ |
| $B$ | Width (channel, fin) | m |
| $Bi$ | Biot number | – |
| $Br$ | Brinkman number | – |
| $c$ | Specific heat capacity (solids, fluids) | $J/(kg \cdot K)$, $kJ/(kg \cdot K)$ |
| $c_p$ | Specific heat capacity at constant pressure | $J/(kg \cdot K)$, $kJ/(kg \cdot K)$ |
| $c_v$ | Specific heat capacity at constant volume | $J/(kg \cdot K)$, $kJ/(kg \cdot K)$ |
| $c_f$ | (Wall) Friction factor (Fanning) | – |
| $C_i, c$ | Integration constant, numerical value | Problem-oriented |
|  | Series expansion coefficient, Chapter 7 | – |
| $COP$ | Coefficient of performance, subscript C: Carnot $COP$ | – |
| $D$ | Diameter | m |
|  | Diffusion coefficient | $m^2/s$ |
| $D_h$ | Hydraulic diameter, Equation 4.23 | m |
| $D_1$ | First series expansion coefficient, Table 7.3 | – |
| $De$ | Deborah number | – |
| $e$ | Equivalent sand roughness, Figure 4.12 | m, mm |
| $E$ | Energy | J, kJ |
|  | Emissive power (radiation), subscript S: black body | $W/m^2$ |
| $E_a$ | Activation energy | J/kmol |
| $E_\lambda$ | Spectral emissive power | $W/(m^2 \cdot \mu m)$ |
| ENE | Net energy effectiveness | – |
| $Ex$ | Exergy | J, kJ |
| $f_G, f_T$ | Geometry, temperature parameters, Table 5.3 | – |
| $F$ | Force | N |
| $F$ | Helmholtz free energy | J, kJ |
| $F(\varsigma)$ | Spatial function, Equation 7.60 | – |
| $F_{ij}$ | View factor, Section 5.7.6 | – |
| $Fo$ | Fourier number | – |
| $g = 9.81 \ m/s^2$ | Gravitational acceleration | $m/s^2$ |

| Symbol | Description | Unit |
|---|---|---|
| $G$ | Gibbs free energy, free enthalpy | J, kJ |
| $G_m$ | Molar Gibbs energy | J/kmol, kJ/kmol |
| $G$ | Shear modulus | $N/m^2$ |
| $G$ | Immissive power (irradiation) | $W/m^2$ |
| $G_\lambda$ | Spectral immissive power | $W/(m^2 \cdot \mu m)$ |
| $G(Fo)$ | Time function, Equation 7.60 | – |
| $Gr$ | Grashof number | – |
| $Gz$ | Graetz number | – |
| $h$ | Specific enthalpy | J/kg, kJ/kg |
| $h$ | Planck's constant | J·s |
| $h_{1+x}$ | Specific enthalpy of moist air, Equation 8.16 | J/kg dry air, kJ/kg dry air |
| $H$ or $h$ | Height, fin length | m |
| $H$ | Enthalpy | J, kJ |
| $H_m$ | Molar enthalpy | J/kmol, kJ/kmol |
| $H_u$; $H_o$ | Lower heating value (LHV); upper heating value (UHV) | J/kg, kJ/kg |
| $H_{mu}$; $H_{mo}$ | Molar heating value, lower; upper | J/kmol, kJ/kmol |
| $i, j$ | Summation indices | – |
| $J$ | Radiosity (radiation) | $W/m^2$ |
| $J_\lambda$ | Spectral radiosity | $W/(m^2 \cdot \mu m)$ |
| $J_0, J_1$ | Bessel function, zeroth or first kind | – |
| $k$ | Consistency factor (power law, Equation 9.2) | Pa·s (Newtonian fluid) Pa·s$^n$ (non-Newtonian fluid) |
| $k$ | Total (or overall) heat transfer coefficient | $W/(m^2 \cdot K)$ |
| $k$ | Reaction rate constant (second order) | $(kg/kmol)^{-1} \cdot s^{-1}$ |
| $KE$ | Kinetic energy | J, kJ |
| $L$; $L_{ref}$ | Length; reference length | m |
| $Le = a/D$ | Lewis number | – |
| $m$ | Mass, subscript L: dry air, W or $H_2O$: water, G: dry solid, B: fuel | kg |
| $m$ | Fin parameter, Equation 6.6 | $m^{-1}$ |
| $m$ | Exponent (power law, Equation 9.1) Exponent (Nusselt correlation, Equation 5.38) | – – |
| $\dot{m}$ | Mass flow rate, subscript B: fuel | kg/s |
| $\dot{m}_{WA}$ | Drying rate (per unit area), Equation 8.38 | $kg/(s \cdot m^2)$ |
| $M$ | Molar mass | kg/kmol |
| $M_t$ | Torque | N·m |
| $Ma$ | Mach number | – |
| $n$ | Molar quantity (number of moles) | – |

| Symbol | Description | Unit |
|---|---|---|
| $n$ | Exponent (power law, Equation 9.2) | – |
| | Exponent (Nusselt correlation, Equation 5.38) | – |
| $n$ | Geometry parameters of heat conduction ($n = 0$: plane wall, $n = 1$: cylinder, $n = 2$: sphere) | – |
| $Nu$ | Nusselt number, subscript m: mean value | – |
| $p$ | Pressure, subscript s: saturation pressure, L: air partial pressure, W: vapor partial pressure | Pa, bar |
| $p$ | Exponent, Table 5.3 | – |
| $PE$ | Potential energy | J, kJ |
| $Pe$ | Péclet number | – |
| $Pr = v/a$ | Prandtl number | – |
| $\dot{q}$ | Heat flux | $W/m^2$, $kW/m^2$ |
| $Q$ | Heat | J, kJ |
| $\dot{Q}$ | Heat rate | W, kW |
| $r$ | Radius (variable) | m |
| $r_0$ | Specific enthalpy of vaporization (water at 0 °C) | J/kg, kJ/kg |
| $R$ | Individual gas constant, subscript L: standard air, subscript W: water vapor | J/(kg·K) |
| $R$ | Radius (pipe, cylinder, sphere) | m |
| $R_i$ | Specific resistance, subscripts: $i = \alpha$: heat transfer resistance $i = \lambda$: heat conduction resistance | $K \cdot m^2/W$ |
| $R_i$ | Surface radiative resistance, Equation 5.96 | $m^{-2}$ |
| $R_{ij}$ | Space radiative resistance, Equation 5.88 | $m^{-2}$ |
| $R_M = 8314.4621$ | Universal gas constant | J/(kmol·K) |
| $R_{th}$ | Thermal resistance, with additional subscript $\alpha$: heat transfer resistance $\lambda$: heat conduction resistance | K/W |
| $Ra$ | Rayleigh number | – |
| Re | Reynolds number | – |
| $s$ | Specific entropy | J/(kg·K) |
| $s$ | Wall thickness (Ch. 5), fin thickness (Ch. 6), half slab half thickness (Ch. 7) | m |
| $S$ | Hole or slot spacing, Figures 5.8 and 5.9 | m |
| $S$ | Entropy | J/K |
| $Sc = v/D$ | Schmidt-number | – |
| $Sh$ | Sherwood-number, subscript m: mean value | – |
| $St$ | Stanton-number, subscript m: mean value | – |

| Symbol | Description | Unit |
|---|---|---|
| $t$ | Time | s |
| $t_e$ | Lifetime | a (years) |
| $t_{Kn}$ | Break point time | s |
| $T$ | Absolute (or thermodynamic) temperature | K (kelvin) |
| $T_g$ | Glass transition temperature | °C |
| $T_m$ | Melting temperature | °C |
| $T_z$ | Decomposition temperature | °C |
| $u$ | Specific internal energy | J/kg, kJ/kg |
| $U$ | Internal energy | J, kJ |
|  | (Wetted) Perimeter | m |
| $v$ | Specific volume | m³/kg |
| $v_{1+x}$ | Specific volume of moist air Equation 8.12 | m³/kg dry air |
| $V$ | Volume | m³ |
| $\dot{V}$ | Volumetric flow rate | m³/s |
| $w$ | Velocity, subscript m: mean value | m/s |
| $w_v$ | Volumetric strain energy, Section 2.5.1 | J/m³ |
| $w_\infty$ | Free stream velocity outside the boundary layer | m/s |
| $\dot{w}$ | Volumetric thermal power, Equation 7.6 | W/m³ |
| $\dot{w}_R$ | Friction power per unit area, Equation 9.30 | W/m² |
| $W$ | Slot width (Figures 5.7 to 5.9) | m |
| $W$ | Work | J, kJ |
| $W_{KV}$; $\dot{W}_{KV}$ | Technical work; technical power (open system) | J, kJ; W, kW |
| $W_{12}$ | Work between states 1 and 2 (closed system) | J, kJ |
| $W_R$ | Friction work | |
| $W_{rev}$ | Reversible reaction work | J, kJ |
| $W_{mrev}$ | Molar reversible reaction work | J/kmol, kJ/kmol |
| $W_V$ | Volume integral, Section 3.2.5 | J, kJ |
| $\dot{W}$ | Mechanical power, subscript R: friction power | W, kW |
| $W_p$ | Reversible technical work or pressure integral, Section 3.3.7 | J, kJ |
| $We$ | Weissenberg number | – |
| $x$ | Humidity ratio of moist air, Equation 8.5 | kg/kg dry air or % |
| $X$ | Humidity ratio of moist solid, Equation 8.31 | kg/kg dry solid or % |
| $x, y, z$ | Position coordinates | m |
| $z$ | Elevation (referred to reference) | m |

# Part 1

# Introductory Fundamentals

# 1  Introduction

## ■ 1.1  The Importance of Energy Technology in Plastic Processing

The main processes for producing plastic materials and manufacturing products made of plastics are shown in Figure 1.1. Due to lower processing temperatures, they are more energy-efficient than processes for producing metal parts. However, most of them are demanding in terms of process engineering. In particular, this applies to procedures called "*Urformen*" in German, i.e., creation of the product shape (primary shaping). Due to their importance compared to the other two common types of plastics, thermosets and elastomers, the *focus is on thermoplastics* in this book.

Temperatures in thermoplastics processing usually are between room temperature and approximately 300 °C, in some exceptional cases up to 400 °C. Common standard plastics have processing temperatures in the range of 200 °C to 250 °C [WK-1]. For several reasons, thermal engineering issues play a dominant role, particularly regarding

- Economy and sustainability (energy requirements, cycle time determined by heating and cooling, future production methods, etc.)
- Product quality (strongly influenced by process control, mainly its temperature curve)

Therefore, it is appropriate to address these issues in more detail in the following chapters and provide the necessary basics for their treatment.

Energy-intensive processes such as injection molding or extruding occur in many variants. Due to the lower processing temperatures, energy requirements in the plastics sector are considerably lower compared to those for processing metals, as mentioned above. Main energy requirements are:

Energy aspects

- Electrical or mechanical energy for drives and movement (pumps, screws, tools, presses, etc.)

- ▪ Thermal or electrical energy for heating and cooling the plastic material, and, for example, for controlling the temperature of tools or calender rollers
- ▪ Electrical energy for welding processes, e. g., laser welding
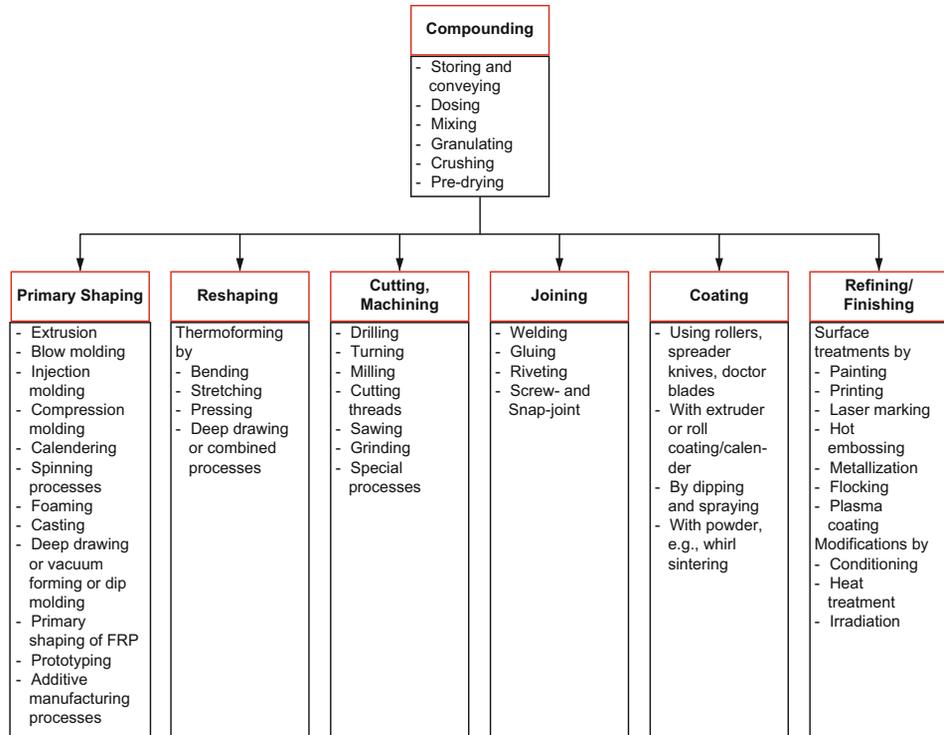


**Figure 1.1**  Manufacturing processes in plastics technology, from [KA-1]

In the case of injection molding, for example, the proportion of energy costs to total manufacturing costs is only about 3% to 5% [KV-1]. This value seems to be very small. However, energy is required several times during plastic processing: heating the granulate, controlling the temperature of the tool, and driving the injection molding machine. Increasing energy efficiency and saving energy are permanent tasks.

Use of waste heat   In modern production plants, the waste heat of manufacturing processes is used for space heating, air-conditioning, or energy storage.

Cycle time   The cycle time has a considerable impact on the economic efficiency of injection molding processes. On the other hand, cycle time is strongly dependent on the heating and cooling times. These, in turn, depend on the intensity of the heat transfer processes.

Quality   The quality of products made of plastics depends strongly on the temperature curve of the machinery (tools, rollers, etc.) – a matter of thermal process control – which, in turn, determines the cycle time.

These few remarks may show that

- interdisciplinary approaches are needed when dealing with energy issues.
- in general, attention should be paid to energy technology.

This is done in practice but often on an empirical basis. Only in recent years have scientific methods been applied for process optimization. Our contacts with machine manufacturers and manufacturing companies show that sustainability in general and resource efficiency in the use of energy and materials, in particular, are of great importance.

In this book, we limit ourselves to fundamentals and their applications required to assess existing systems (analysis) and identify measures for improving the energy efficiency of plastic process design. We do not address questions of machinery design, design of their components (dies, screws, molds, etc.), electrical engineering, and control technology.

The behavior of plastics in the solid and molten states is much more complex than that of metals, especially with regard to elastic, viscous, and caloric behavior. Chapters 2 and 4 deal with these topics.

## ■ 1.2 Plastic Processing Stages

Figure 1.2 shows the sequence of general plastic processing stages for thermoplastics [KV-8]. Three thermomechanical processing steps are relevant:

- *Melting stage*: The plastic, initially in a solid state, either as a powder or as a pellet, is converted to a molten state. Depending on the type of plastic, semi-crystalline or amorphous, different physical phenomena influence the energy required for the melting process.
- *Shaping stage*: A specified shape is imposed on the molten plastic by injecting or blowing it with pressure into a mold or through a die.
- *Third stage*, where the final shape of the (solid) product is achieved by drawing, stretching, or blowing and eventually by cooling.

Energy in different forms is required in all processing stages.
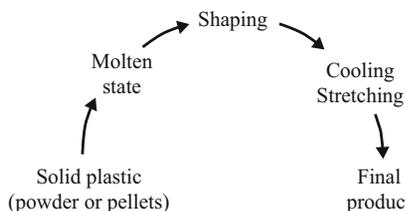


**Figure 1.2**
Plastic processing stages, from [KV-8]

# ■ 1.3 Logic for Processing Design

Plastics have specific properties that are decisive for the processing design. The following explanations are taken from [KV-8], partially from [KV-9].

### Thermally Insulating Character of Plastic Melts

The *thermal conductivity* of plastic melts is on the order of magnitude of 0.2 W/(m·K) only, which means two to three orders of magnitude lower than that of metals, leading to high cooling or heating times. According to the basics presented in Chapter 7, cooling and heating times increase with increasing wall thickness, approximately with the second power. The orders of magnitude are:

| Wall thickness | Cooling or heating time |
| --- | --- |
| 0.1 mm | 0.1 s |
| 1 mm | 10 s |
| 10 mm | 1000 s |

*This shows that melting a polymer by unique conduction from equipment walls would lead to unacceptable long residence times and low flow rates. That is why all melting processes require significant mechanical energy input, often much more extensive than thermal energy transferred by conduction. The low thermal conductivity also implies that the majority of plastic products are less than a few millimeters thick to minimize the cooling times and favor high production rates [KV-8].*

### Very High Viscosity of Plastic Melts

Under typical processing temperatures, molten plastics have viscosities of about $10^3$ Pa·s, a million times higher than that of water. The practical consequences are:

- *Reynolds numbers* – representing the ratio of inertia to viscosity terms, see Chapter 4 – are extremely low. Therefore, the flows of molten plastics are never turbulent, and the inertia terms are usually negligible.

- Heating plastics in the barrel of an extruder or an injection molding machine is achieved by viscous dissipation and electric heating.

- *High pressures* are required to ensure the flow of plastic melts in dies and molds at high flow rates, typically 100 MPa or more for injection pressures, 5 to 50 MPa in extruders.

**Combined Insulating Character and High Viscosity**

The combination of high viscosity, viscous dissipation, and low thermal conductivity creates large temperature gradients in plastic melt flows. Increased local temperatures can lead to the degradation of the plastic. Therefore, viscous dissipation and applied flow rates need to be limited. In some cases, the viscous dissipation dominates so that even cooling is necessary, a step to avoid plastic degradation. However, this is a step to be avoided in the interest of energy efficiency [KV-2].

*On the other hand, the high viscosity of polymers coupled with their low conductivity allows us to design processes in ambient air where extrudates remain in the molten state before going through shaping devices or drawing systems. These properties have led to the development of many downstream extrusion processes: spinning, blowing, stretching [KV-8].*

**Sensitivity of Viscosity to Shear Rates and Temperature**

*Typically, the viscosity of a molten polymer may decrease by a factor of five when the shear rate is increased by a factor of ten, and it may drop by a factor of two when the temperature is increased by 20 °C [KV-8].*

The high sensitivity of viscosity to the shear rate and temperature significantly impacts flow behavior and process optimization.

**Viscoelasticity**

A plastic may behave as a liquid or a solid depending on temperature and the speed at which the molecules deform. This behavior, which ranges between liquid and solid, is referred to as the viscoelastic behavior. Viscoelasticity refers to the combination of viscous and elastic material properties. *Linear viscoelasticity* is limited to plastic systems undergoing small or slow deformations, whereas *nonlinear* viscoelastic models are required for large and rapid deformations [KV-9].

In plastic processing, viscoelasticity plays many roles, such as:

- It stabilizes the drawing or biaxial stretching of plastic melts, thus allowing spinning at high strain rates, blow molding, and thermoforming with homogenized thicknesses.

- It may be the origin for the onset of instabilities in shear flows.

- It is responsible for the swelling at the outlet of dies.

In Chapter 2 we cover a few aspects of viscoelasticity. Simple linear viscoelastic models provide some basic understanding of the behavior of plastic materials during deformation.

# ■ 1.4 Required Fundamentals

## 1.4.1 Overview

Figure 1.3 provides an overview of the necessary basics of thermodynamics, fluid mechanics, heat transfer, and material behavior, especially the complex flow and stress–strain behavior of plastic melts (rheology) in plastic processing. In this book, we cover the basics of these disciplines, which we believe to be relevant in the context of plastic processing. For further details, the reader is referred to selected standard textbooks:

- Thermodynamics          In English: [TH-3 to 5]    In German: [TH-1, 2]
- Fluid mechanics         In English: [FM-2]          In German: [FM-1]
- Heat and mass transfer  In English: [WU-2, 3]      In German: [WU-1, 4, 5]

Information on material behavior, including material data, is provided in Chapter 2.

**Fluid mechanics**
- Conservation of mass, impulse, momentum
- Equilibrium conditions
- Flow behavior (rheology)
- Shear and elongational flows

**Thermodynamics**
with its 4 main laws:
0: Thermal equilibrium
1: Conservation of energy
2: Entropy as state property "quality of energy": exergy and anergy (energy = exergy + anergy)
3: Reference state of entropy = 0

**Thermal process engineering focusing on production processes for plastics**

**Heat transfer**
by
- Heat conduction
- Convection: forced and free convection
- Radiation
- Their combinations

**Behavior of materials**
- Thermal & caloric equations of state
- For dealing with thermal process engineering; relevant material data for gases, liquids (in particular: coolants), thermoplastics, cross-linked elastomers, thermosets
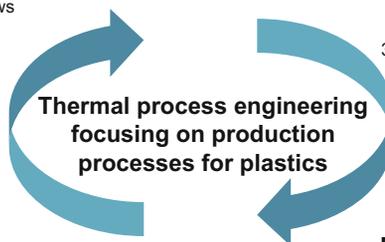
**Figure 1.3** Interaction of the disciplines thermodynamics, fluid mechanics, heat transfer, and material behavior required in thermal process engineering

Besides heat transfer, mass transfer is required for treating processes such as mixing, degassing, and pre-drying. To limit the volume of this book, we do not cover the fundamentals of mass transfer. Instead, we refer to the standard textbooks mentioned above. Similarly, in Chapter 8, which provides an overview of drying

processes, we only deal with the basics necessary for treating simple drying processes under ambient air conditions.

The abovementioned basic disciplines are treated individually with partial overlaps in standard textbooks. Figure 1.3 illustrates that solving practical engineering problems requires an interdisciplinary approach. A recommended introductory book on thermal systems engineering, [VT-2], covers the basics of thermodynamics, fluid mechanics, and heat transfer in an integral way.

Thus far, the remarks refer to thermal process engineering, i. e., processes without chemical reactions. A well-known German-language book on this subject is [VT-1]. There are also processes with chemical reactions in plastics processing, e. g., combustion or polymerization processes. In that case, we are talking about chemical process engineering; see, e. g., [VT-3].

Many chemical process engineering textbooks deal with reaction kinetics rather than energy rate balances relevant in energy technology. To limit the scope of this book, chemical reactions are covered only marginally in Chapter 3, Section 3.5.

The following chapters of Part 1 provide introductory explanations, key definitions, and basic principles of thermodynamics, fluid mechanics, heat transfer, and behavior of plastic materials. Extended fundamentals for practical purposes are covered in the chapters of Part 2. *End-of-chapter examples*, called basic examples, illustrate the application of basic principles of Parts 1 and 2. The *practical examples* of Part 3 intend to illustrate the interdisciplinary approach in solving problems of some fundamental processes of Figure 1.1. They all have been worked out jointly with industrial companies, machine manufacturers, and manufacturers of products made of plastics. To finish this introduction, we address three relevant issues:

- System analysis
- Kinds of systems
- Methodology for solving engineering problems

## 1.4.2 System Analysis

The critical step in any technical analysis is the precise description of what is to be analyzed, i. e., the proper definition of the system.

To illustrate the procedure, we will deal with a simple and illustrative example from mechanics. When examining the static and dynamic behavior of mechanical components (stress and strain levels, motion, etc.), the first step is always to create the so-called free body diagram of the element to be analyzed.
Mechanics

The body is completely isolated from its surroundings. In mechanics, the term "free body diagram" is used for the *isolated body*, the system under consideration.
Free body diagram

At the boundaries with the surroundings, *all* acting forces and moments are introduced. Then,

- the conditions of equilibrium → static cases
- Newton's laws of motion → dynamic cases

are formulated. We illustrate the methodology with the simple example of a rotary crane; Figure 1.4. The object of study shall be the crane's boom. We are interested in all forces acting under stationary conditions. It is of utmost importance that *all forces* and *moments,* known and unknown, are entered in the free body diagram, the isolated boom (in blue in Figure 1.4). They represent the *mechanical interaction* between boom and surroundings.
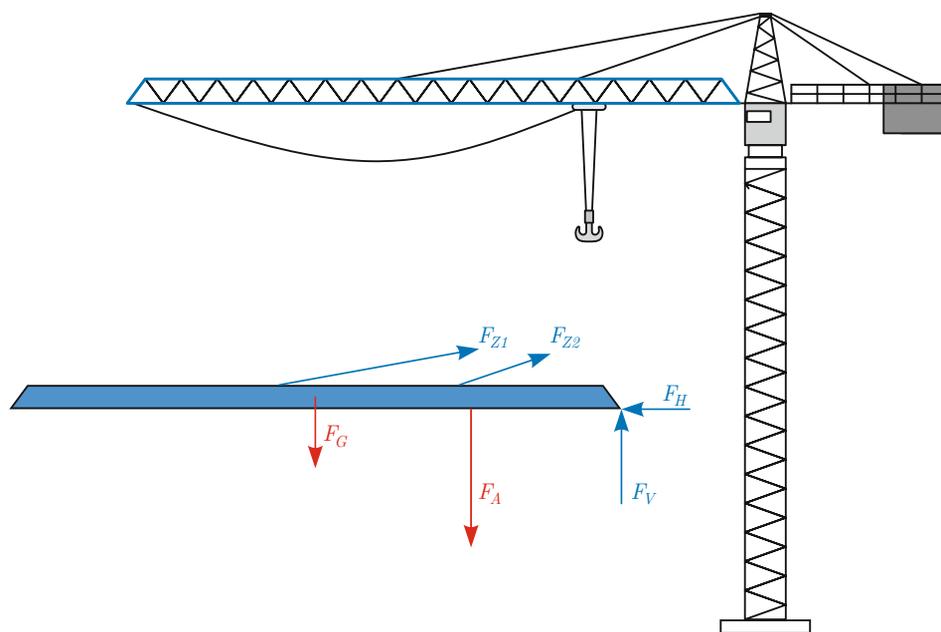
**Figure 1.4**  Rotary crane: free body diagram of the component to be analyzed, the boom

In reality, the weight $F_G$ is a distributed load (track load); for simplifying reasons, we introduce it as a single load (point load). $F_A$ represents the horizontally sliding towing load. Both forces $F_{Z1}$ and $F_{Z2}$ describe the interaction with the tensile rods attached to the top of the crane tower. The effect of the joint on the right-hand side is specified by the horizontal and vertical bearing reactions, $F_H$ and $F_V$. The bearing moment is of minor importance; therefore, we neglect it here.

Taking account of the weight of the rope cables depends on the objectives and the accuracy requirements of the analysis. A possible simplification could be to add the weight of the left-hand part of the hanging rope to the boom's weight and the weight of the right-hand portion to the towing load.

*Known forces* are the weight $F_G$ – including the weight of the hanging rope – and the amount and the position of the sliding towing load $F_A$. The remaining four forces, $F_{Z1}$, $F_{Z2}$, $F_H$, and $F_V$, are *unknown*. For solving this two-dimensional problem, *three equilibrium conditions* can be formulated, *one* moment relation and *two* force relations – one in the horizontal and one in the vertical direction. Therefore, the problem is onefold statically indeterminate, i.e., we need an additional relationship, which can be obtained by considering the deformation conditions of the two tensile rods. If the boom is assumed to be rigid, the elongations of the tensile rods are in a fixed ratio given by the geometry. This ratio also applies to the ratio of the forces $F_{Z1}/F_{Z2}$, assuming linear-elastic deformation (Hooke's law). This deformation condition gives an additional equation. All external loads acting on the boom are determinable. With known load conditions, stresses and deformations (deflections, elastic curve) can be determined. Of primary interest are locations of maximum stress and deflection.

In thermal systems engineering, with disciplines thermodynamics, fluid mechanics, and heat and mass transfer (Figure 1.3), the terms "*system*" and "*control volume*" are used instead of the term "free body diagram" used in mechanics. However, their role is the same in both cases, namely, the precise definition of the subject of the analysis. We say without exaggeration: | System concept

> ❗ The system concept plays an equally important role in energy technology as the function concept in mathematics.

As shown with the simple mechanical example, the initial step in any engineering analysis is to precisely define what is to be analyzed, the *system definition*. The system is separated from the surroundings by the *system boundary*. Everything inside the system boundary belongs to the system; everything outside belongs to the surroundings. | System boundary

Just as all forces and moments are entered in the free body diagram, all relevant *interactions between the system and the surroundings* are formulated at the system boundary and entered into the system sketch. These interactions are more diverse than in mechanics; for example, they include mass flows, heat flows, mechanical and electric power which may cross the system boundary at different locations. The analog to formulating equilibrium conditions or Newton's laws of motion in mechanics is the formulation of the *rate balances*, primarily for the conservation quantities mass, momentum, angular momentum, and energy. | Interaction with the surroundings

> ❗ Fundamental steps when formulating rate balances for energy, mass, etc. are:
> - Proper definition of the system
> - Precise definition of the system boundary: What belongs to the system under consideration? What belongs to the surroundings?
> - Complete description of the interaction between system and surroundings, i.e., formulation of all mass and energy flows crossing the system boundary

The system can be complex like an entire injection molding machine (Figure 1.5) or simple like a heat exchanger. It can also be a differential volume element when dealing with numerical methods for determining flow or temperature fields.
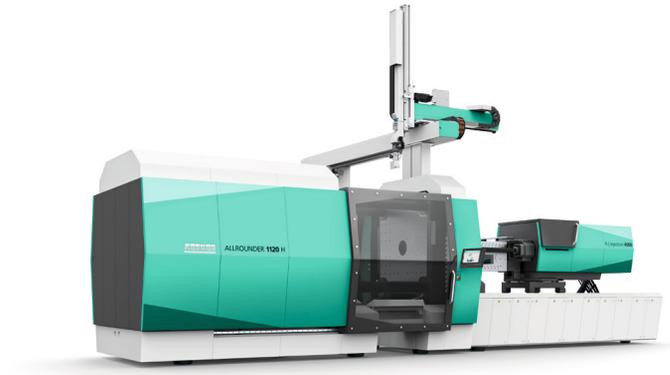


**Figure 1.5**  Injection molding machine (image: Arburg GmbH + Co. KG)

System    The system is a mental aid for problem analysis. It is a physical structure separated from the surroundings by an imaginary *closed surface* – the system boundary – completely enclosing the system.

Control volume KV    When mass crosses the system boundary, the term "control volume" (*Kontrollvolumen* in German, abbreviated KV) is preferred for the region enclosed by the system boundary. The system boundary can be fixed or movable.

The appropriate choice of the control volume and system boundary, respectively, will depend on the type of problem to be solved. If the focus is on the energy budget of the entire injection molding machine, the system boundary is set around it. If the main interest is in the screw (granulate in, plastic melt out, heating, and driving power), an appropriate choice of the system boundary enclosing the screw would be along the inner surface of the barrel.

The system boundary should be placed so that the surroundings' interactions can be described as precisely as possible. The art of selecting an appropriate and problem-oriented system boundary is a matter of experience.

An undeniable advantage of the system approach is that, at least for steady-state conditions, one does not have to worry about the details of complex processes within the system boundary. If it is possible to describe what happens at the system boundary with some degree of reliability, i.e., which mass and energy flow across the system boundary, the balance equations provide access to quantities that cannot accurately be measured or computed with reasonable effort.

### 1.4.3  Kinds of Systems

Depending on the problem to be solved, different system kinds are common in energy technology. The most important ones are *open*, *closed,* and *adiabatic* systems.

A system is open when energy and mass flows cross the system boundary. Keep in mind that mass flows, besides transporting mass, also transport energy. Section 3.3 deals with the first law of thermodynamics for open systems, where the property *enthalpy* will be defined. The transfer of thermal energy associated with a mass flow is called *convective thermal energy transfer*. Most systems in practice are open systems, for example, the tool of an injection molding machine whose temperature is controlled by oil or water flows.

Open system

A system is closed if its boundary is *impermeable to mass*, i.e., the system's mass remains constant during the process under consideration. However, energy may cross the system boundary as heat and work. Example of a closed system: air inside a piston–cylinder assembly (displacement volume) of a piston engine with closed valves and dense piston rings. Energy transfer by work happens by moving the piston during the compression cycle. Energy transfer by heat takes place across the cylinder walls.

Closed system

A system is adiabatic if its entire system boundary is *impermeable to heat*. Energy transfer may take place by work and/or mass flow only. In other words, adiabatic systems may be open or closed without heat transfer across its system boundary. The system boundary of a nonadiabatic system can be partially adiabatic. Adiabatic systems and adiabatic system boundaries are idealizations.

Adiabatic system

### 1.4.4  Methodology for Solving Thermal Systems Problems

We strongly recommend adopting a proven systematic approach for solving thermal systems engineering problems. The methodology described here is used in English-language textbooks (e.g., standard textbooks by publishing companies such as John Wiley & Sons and McGraw-Hill, in particular, the excellent books [TH-3, 4, 5], [FM-2], [WU-3], and [VT-2]), but also increasingly in the German-speaking area, e.g., [WU-4, 5]. We call it *a six-point solution methodology*. Of course, it may be supplemented by additional sections or points without changing the essence of the methodology.

**1. Known (Given Data)**

What do we know about the problem? What quantities are given or specified? Trying to answer these questions, studying the problem, and reflecting on the occurring processes are an integral part of the problem analysis.

### 2. Find

What does one want to know about the problem? What is to be determined? Jointly with step 1, consider what properties are to be determined, what transfer processes take place, and what relationships are involved. Points 1 and 2 should provide a comprehensive definition of the problem.

### 3. System and Schematic Diagram

Select the system appropriate to the problem. Set the system boundary so that the interaction with the surroundings can be expressed reasonably. Think about where one wants to determine quantities obtainable via the balance equations. Clear identification of the *interaction with the surroundings* is a relevant issue of this step. Consider what change the system undergoes: Is the process stationary or subject to changes in time? We strongly recommend sketching the system (→ schematic diagram) and entering *all* mass and energy flows at the locations where they cross the system boundary. All given properties should be listed as well.

**Example B 1.1** (Section 1.5) illustrates the interaction of a simple system with the surroundings for two different system boundaries.

### 4. Simplifying Assumptions

In general, technical systems and their interaction with the surroundings are complex, and their modeling needs to be simplified. Examples: one-dimensional flow, uniform pressure distribution, adiabatic walls, neglecting heat flows due to radiation, etc. It is advisable to list *all* simplifying assumptions and idealizations made. With this step, develop a suitable engineering model.

### 5. Analysis

In this step, equations are formulated, i.e., the balance equations for mass, energy, momentum, and, if necessary, angular momentum and other fundamental laws. We strongly recommend

- performing the analysis algebraically before introducing numbers,
- substituting numerical data after establishing functional relationships. Only in this way does the influence of the individual parameters become transparent,
- checking relationships and data for dimensional homogeneity,
- subjecting intermediate and final results to a plausibility check: Are the magnitudes of the numerical data reasonable?

In summary, the essential analysis steps are:

- Select an appropriate *coordinate system.*

- Define *boundary conditions*, and in the case of transient processes, define *initial conditions.*

- Specify *all interactions* of the system with the surroundings in conjunction with the boundary conditions.

- Depending on the problem to be solved, different laws are required, e. g., Fourier's law of heat conduction, material laws specifying the relationship between stress and strain for solid materials, describing viscosity for fluids, etc.

- Formulate *balance equations* for mass and energy (also for momentum and angular momentum if required) using the selected coordinate system.

- Solve equations or system of equations for quantities to be determined (flow field, temperature field, energy flows, etc.) and – if appropriate – graphically represent them.

- Take *material data* from relevant databases. For details, see Chapter 2. Because of plastics' enormous diversity and complexity, getting consistent data for solids and melts is still a real challenge.

### 6. Discussion

Following the analysis, the results obtained need to be judged in this step. In particular, one should examine to what extent the simplifying assumptions are appropriate and whether they need to be adapted. Is the choice of the system, including its boundary, reasonable? For complex problems, a first analysis using simplifying assumptions provides a "feeling for the order of magnitude" of the parameters involved, thus making it possible to specify more accurate assumptions for a second or even a third analysis step. This so-called *successive iteration procedure* is typical for engineering problem-solving in practice. In short, the methodology is:

- Perform a comprehensive problem assessment (steps 1 to 4) first.

- After that, perform the analysis, formulate and solve equations, and evaluate the results (steps 5 and 6). If necessary, add further iteration steps.

The sample solutions of all examples, the *basic examples* following each chapter of Parts 1 and 2 as well as the *practical examples* of Part 3, are treated using this methodology. It represents a way to model reality mathematically. This type of modeling is called *process simulation*, performed analytically or numerically.

In general, the analytical method requires simplifying assumptions. However, it does provide the essential relationships in the correct order of magnitude with comparatively little effort. Thus, if necessary, i.e., when higher accuracy results are required, the analytical method represents the starting point for more detailed investigations, like experiments or numerical simulations using advanced simulation tools.

*Analytical method*

Numerical method  Numerical methods (finite difference method, FDM, or finite element method, FEM) are more complex; on the other hand, they allow a more realistic system modeling. Both methods, analytical and numerical, have their justification and are in use in plastics technology today.

In this introductory textbook, we limit ourselves to the analytical method. The analytical solutions – that is, their numerical results – of all examples are obtained using the software package Maple™.

# ■ 1.5 Example B 1.1: Interaction with the Surroundings for System Boundaries A and B of System "Extruder"
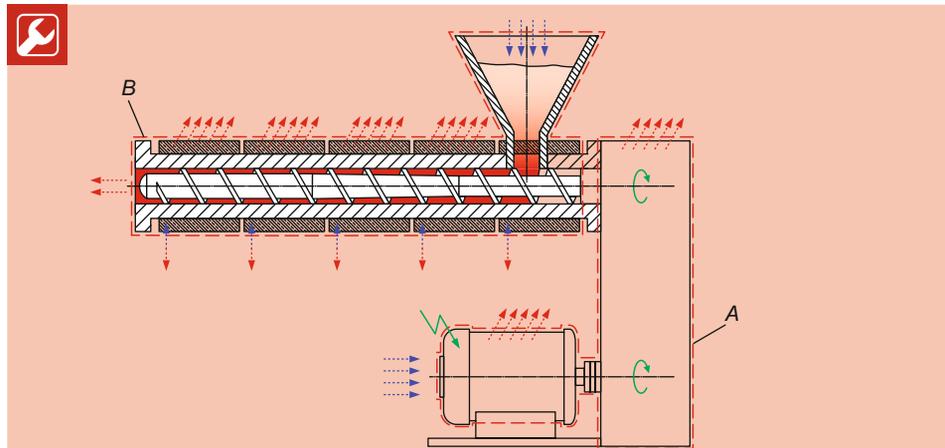


**Figure 1.6** System "extruder" with system boundaries A and B [KA-1]

**System boundary A "drive system" includes an electric drive motor, closed belt drive, and gear**

- Mass flows (note that the system boundary is placed on the surface of the elements): cooling airflow for cooling the drive motor; air enters with ambient air temperature and leaves system A at elevated temperature, thus transferring thermal energy to the surroundings
- Energy flows: electric power to drive motor → in, mechanical drive power to extruder screw → out
- Heat flows: heat transfer motor/belt/gear casing → surroundings due to free convection and radiation
- Convective thermal energy transfer by the motor cooling air, as mentioned above

**System boundary B includes funnel, hopper, and extruder**

- Mass flows: granulate supply, extrudate at the outlet, heating and cooling fluid mass flow for temperature control
- Energy flows: mechanical power to extruder shaft, heating and cooling power (barrel), heat transfer barrel → surroundings due to free convection and radiation
- Convective thermal energy transfer by the plastic (granulate in, extrudate out)

Note that in both systems, convective energy transfers take place associated with mass flows.

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# 2 Material Behavior of Plastics

Compared to other classes of materials, plastics are characterized above all by a unique variety of properties (such as crystal clear or opaque, tough or soft, nonconductive or conductive) that they offer for a wide range of applications. The Latin expression "*mixtura miraculosa*" would therefore be much more appropriate than the word plastic, which is derived from the Greek term *plastikos*: to form/shape. But all joking aside, almost all plastics exist usually as **complex mixtures**!

For a better understanding of plastics, the following "word equation" – also called the main theorem of plastics technology – has a key function in the field of plastics engineering, especially in solving upcoming problems:

> ⚠ *Polymer raw material(s) + Additive(s) → Plastic*

Main theorem of plastics technology

The arrow symbol indicates the process steps of preparation/processing.

In addition, the transparency of this simple statement is complicated by the fact that in everyday life the same designations are used for the polymer raw material(s) ("polymer") as well as for the plastic – for instance, polyethylene terephthalate (PET) in use for bottles.

Last but not least, it should be remembered that this mixture of substances has been prepared with great care. So even the smallest changes (of any kind) in the mixing ratio of the two components must be expected to have profound consequences for the plastic in question.

Finally, among the many topics available on the material behavior of plastics, a strict selection was made on the premise that the following text would at least indirectly maintain the reference to energy.

### The Most Important Facts in Brief

Anyone wishing to understand plastics, their properties, processing, and applications right through to recycling from the ground up must be familiar with their chemistry. Right at the beginning of this chapter, therefore, the aim is to convey as

simply as possible the basic chemistry required for the content of this book, Section 2.1. Armed with this prior knowledge, the focus shifts from chemistry to physics including energetic behavior, Section 2.2.

The focus is now on the behavior of the various types of plastics in the solid and viscous or "molten" states and their dependence on temperature and time. In this context, *thermodynamic properties* become very important not only for this book, but mainly because of their central influence in dealing with plastics, Section 2.3.

Furthermore, the sustainable development goals (SDGs) for the future of plastics cannot be achieved without adequately considering the influence of energy in the form of heat and light – often combined with oxygen – on components or semi-finished products. This is illustrated in a separate section using the example of the ageing of plastics, Section 2.4.

At the same time, it should be recalled once again that in the case of plastics, both the polymer raw material(s) used and the finished blend with additives are almost invariably given the same designation.

This chapter is rounded off with the topic of strain energy and elasticity of solid plastics; see Section 2.5.

# ■ 2.1 Chemical Basics

Macromolecule A broader understanding of the material behavior of plastics requires basic information about the different structure of polymers compared to other materials, for example, metals. In the structure of metals, atoms are considered as their smallest building blocks, which are arranged in atomic lattices. If we compare water, $H_2O$, or carbon dioxide, $CO_2$, with a polymer at this point, the smallest building block common to all is the molecule. But polymers, in contrast, have molecules with at least 1000 atoms being involved, as the lowest limit. The term *macromolecule* is used to take this characteristic into account. However, not only the macromolecule alone but also the *chemical elements* involved in its structure are of fundamental importance for the material behavior of the plastic in question. In addition to the chemical element carbon, these are, above all, hydrogen, oxygen, and nitrogen, all of which belong to the lightweights due to their atomic structure and together explain the *low density of polymers*; see Section 2.2.1.

### Chemical Synthesis

As far as the chemical synthesis of macromolecules is concerned, there are many different possibilities; see Figure 2.1.

**Figure 2.1** Classification of polyreactions, from [KA-1]

One of them is called *chain growth reaction,* which is explained in Figure 2.2 using    Chain growth reaction
the simple example of the generation of the macromolecule polyethylene. The
starting material is the *monomer ethylene* (ethene). By "splitting" its double bond,
many monomers can form a chain (macromolecule) together.



From E to PE

**Figure 2.2** Simplified representation of a chain polymerization from monomer to polymer
using the example of polyethylene

A *pure polymer* (polymer raw material) thus consists, in the simplest case, of a mul-
titude of chemically identical macromolecules, whereby, depending on the type of
plastic, special spatial arrangements are formed, for instance, linear chains or in
helix form.

## 2.1.1 Polymer Raw Material(s)

First of all, the influence of a polymer raw material ("polymer") is to be discussed    Influence of the
using the example of *polypropylene, PP.* Propylene, P (monomer), can be converted    molar mass
into a polymer with different properties during polymerization to polypropylene
(polymer raw material) by different manufacturing conditions such as pressure

and temperature, but especially by highly specific catalysts. Thus, using the example of PP, the same polymer raw material is obtained with variable molar masses or molar mass distribution; see Figure 2.3.



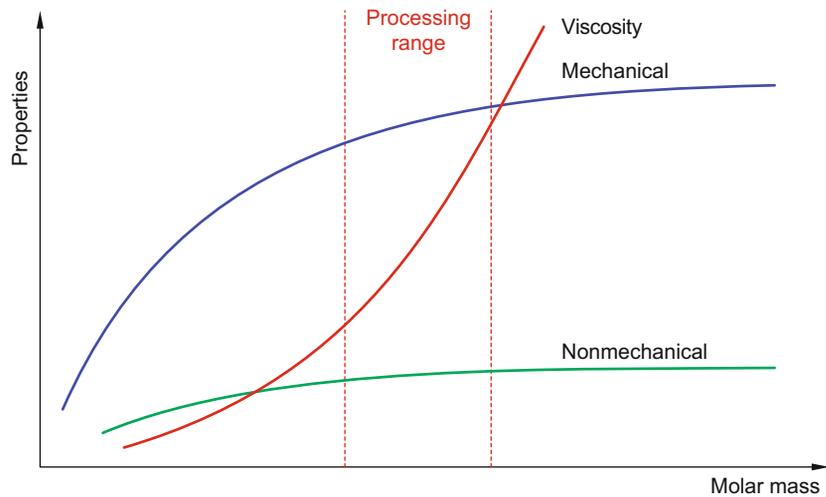**Figure 2.3**  Influence of the average molar mass on physical properties in schematic representation, from [KA-1]

Bimodal distribution    If the specific advantages of both low and very high molar masses are to be combined, the production of a plastic with *bimodal distribution* of the polymer molar mass is an option; see Figure 2.4.
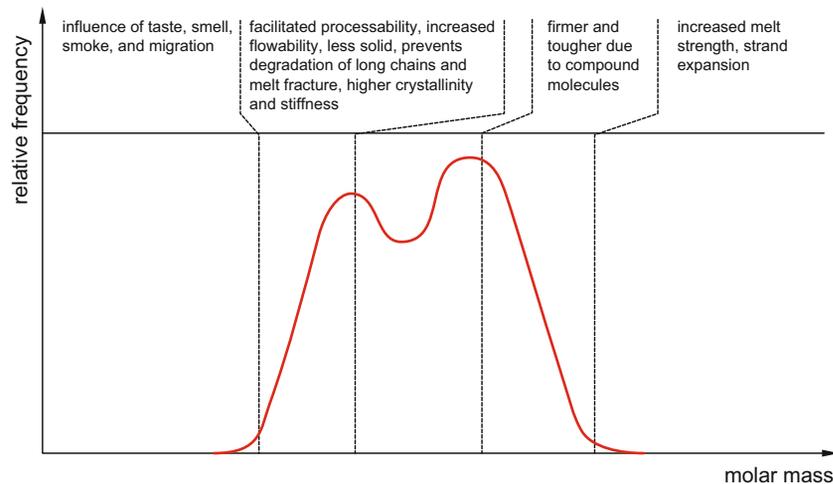


**Figure 2.4**  Schematic of a bimodal distribution curve, from [KA-1]

Further possibilities to obtain "tailor-made polymers" for practical use are offered by the numerous variants of *chemical modification of polymers.* This is achieved, in the case of PP, for example, through the use of additional monomers, e.g., ethylene. Under the generic term "*PP copolymers,*" they find a wide range of applications; see Figure 2.5.
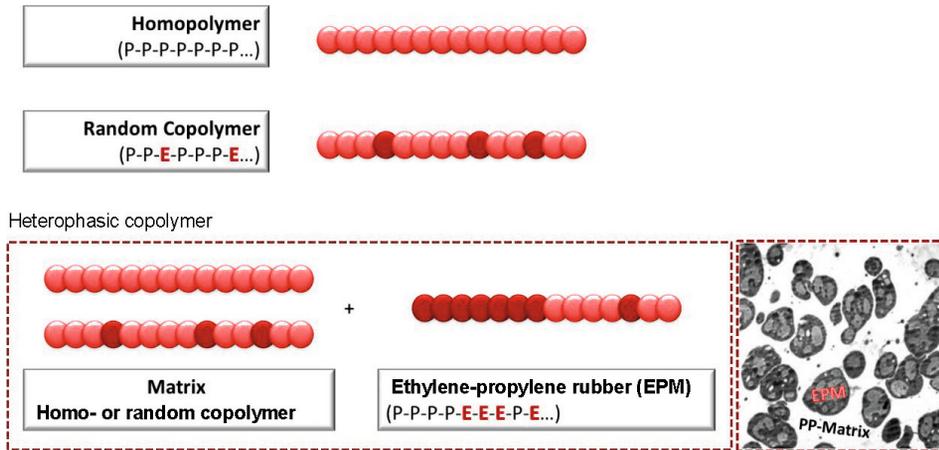


**Figure 2.5**  Schematic structure of propylene copolymers, from [KA-1]

Last but not least, further chemical modifications can be made to the finished polymer raw material. One example is the subsequent chemical cross-linking of thermoplastics.

It should be noted at this point that the possibilities of "tailoring" a polymer raw material that have been described so far and those that follow do not claim to be exhaustive, but – as already mentioned – are to be understood only as *typical examples.*

It is also deliberately intended in Section 2.1 to largely dispense with chemical and physical formulae in the *further description of the material behavior* and instead to give priority to the qualitative approach with words and pictures.

## 2.1.2  Additive(s)

Similarly, the properties of a plastic for its intended use in practice can be permanently changed by a selective choice of additives. In everyday plastic applications, these additional possibilities of *physical modification* are almost always exploited to produce high-quality components or semifinished products (pipes, sheets, profiles, etc.), mostly in combination with the already-mentioned chemical variants to optimize the polymer raw material.

Physical modification

Using several examples – initially as undesirable effects – physical modification will also be explained in more detail. PP, for example, is *hydrophobic* when used as a plastic due to its chemical structure. The situation is completely different with PP reinforced with glass fiber. The physical phenomenon of the wettability of glass fibers by water film ($H_2O$) therefore requires *controlled pre-drying* even before processing in the melting process; see Chapter 8. Otherwise, the desired improvement in mechanical properties would lead to a fault in the component due to water vapor formed as a result, e.g., formation of streaks and bubbles. Polyethylene terephthalate (PET) behaves even more extremely in processing, for example, in the injection molding of preforms used to produce PET bottles. Even as an unreinforced polymer raw material, it is susceptible to *hydrolysis* in the presence of even the smallest traces of water, due to its polyester structure, and consequently requires *extreme pre-drying* before processing. In complete contrast, a polyamide, e.g., PA 66, only acquires its toughness through the absorption of water as an external plasticizer.

Consequential color change — Moreover, for example, a color change in the same plastic, e.g., from green to red, can lead to unforeseen consequences such as *shrinkage behavior*.

The modification of the polymer raw materials with additives takes place, depending on the requirements for the plastic part in question, either already at the polymer raw material manufacturer (producer) and/or during compounding or at the processor. Table 2.1 summarizes the individual requirements for additives. At the same time, this list provides a simple explanation for the huge variety of different plastic products that are encountered in everyday life.

Recycling of plastics — On the flip side, however, this forces all parties involved to pay due attention to plastics recycling from as early as the development stage of new products in the future.

Taking into account new scientific findings and improved technologies in the field of plastics technology, further growth in the plastics industry can therefore be expected worldwide.

**Table 2.1** Thematic Overview: Additives for Plastics (Selection), from [KA-1]

| Reaction substances | Processing-enhancing additives | Strength-increasing additives | Stiffness-increasing additives | Stiffness-decreasing additives |
|---|---|---|---|---|
| ▪ Hardeners (cross-linkers)<br>▪ Photo-initiators<br>▪ Catalysts<br>▪ Accelerators<br>▪ Propellants (for foams)<br>▪ Degradation-causing additives | ▪ Stabilizers (against heat)<br>▪ Antioxidants<br>▪ Lubricants<br>▪ Bonding agents for filling materials, fibers, etc.<br>▪ Nucleating agents<br>▪ Antistatic agents<br>▪ Release agents | ▪ Reinforcements like fibers, fabrics, mats<br>▪ Fillers with reinforcer effect (e. g., carbon black, silica for elastomers)<br>▪ Resin carriers for thermosets (e. g., wood flour, cellulose) | ▪ Reinforcements like fibers, fabrics, mats<br>▪ Fillers without reinforcer effect (e. g., silicon flour, rock flour) | ▪ Plasticizers<br>▪ Rubber-like polymers, mixed into the softening plastic (so-called polyblends, e. g., nitrile rubber in PVC or chlorinated PE in PVC) |
| **Antimicrobial additives** | **Lifetime-prolonging additives** | **Coloring additives** | **Properties-modifying additives** | **Cheapening additives** |
| Biostabilizers against biological attack (e. g., fungistatics against fungus) | Stabilizers against light, oxidation, heat (also called anti-ageing agents) | ▪ Pigments<br>▪ Dyes<br>▪ Brightening agents (e. g., fluorescent brighteners for PVC) | ▪ Flame retardants<br>▪ Heat-conduction-improving additives (e. g., metal powder)<br>▪ Antistatics | Cheap fillers (e. g., slate flour, chalk, etc., so-called stretching agents) |

For a more in-depth understanding of the chemical and physical influences discussed so far – especially with regard to the properties of a plastic – the reader is referred to the relevant technical literature.

## 2.1.3 Classification of Plastics

Plastics can be classified according to a wide variety of criteria, e. g., according to their production, recyclability, areas of application, etc. The *main criterion*, however, remains the following: their different behavior at *elevated temperature*. Thus, two types can be defined initially:

Temperature as a guideline

- Non-cross-linked plastics
- Cross-linked plastics

In the case of non-cross-linked materials, plastic shaping is possible several times through heating. In contrast, cross-linked ones are irreversibly "hardened" into a molded material after passing through their plastic state once during molding and do not soften again when subsequently heated.

The classification of plastics predominantly used in practice goes one step further and is based on the differences in thermomechanical behavior; see the explanations in Section 2.2.1.3.

Three types of plastics can thus be schematically described:

- Thermoplastics and thermoplastic "elastomers"
- Elastomers
- Thermosets

Since thermoplastics account for by far the largest share of global plastics consumption, the following explanations are limited primarily to this class of materials.

### 2.1.4  Bonding Forces in Macromolecular Systems

Shape of a macromolecule

First of all, the question of by which shape a macromolecule can be described in the simplest case must be answered. As a rule, carbon (C) appears as the central chemical element, and C atoms – usually connected to each other by *single bonds* – can form very long chains. The smallest unit of a polymer thus has a thread-like shape, which already explains the *anisotropic behavior* of most plastic components. Parallel to this, the question as to the nature of the bonding forces within a "filamentous" macromolecule and *between neighboring* macromolecules arises.

#### 2.1.4.1  Main Valence Bonds

Chemical bonds

Main valence bonds are chemical bonds. The most important partners in this type of bond between neighboring atoms are, in addition to the already-mentioned carbon, C (quadruple bond), the atoms of hydrogen, H (single bond); oxygen, O (double bond); nitrogen, N (triple bond); as well as sulfur, S (double bond); chlorine, Cl (single bond); and fluorine, F (single bond).

Main valence bonds (also called atomic, electron-pair, homopolar, and *covalent bonds* are used to link monomers to polymers (macromolecules) or to chemically cross-link macromolecules with each other. The bond energy is given in kJ/mol, referred to as dissociation energy: it is the energy that must be supplied to a main valence bond in order to cleave it. Table 2.2 contains bond energies as well as the corresponding bond distances.

**Table 2.2** Bond Distances and Bond Energies of Covalently Bonded Atoms, from [KA-1]

| Bond partners | Bond distance [nm] | Bond energy [kJ/mol] |
| --- | --- | --- |
| C–C (aliphatic) | 0.154 | 347 |
| C=C (aromatic) | 0.139 | 410 |
| C=C | 0.135 | 614 |
| C≡C | 0.120 | 811 |
| C–H | 0.109 | 414 |
| C–O | 0.143 | 351 |
| C=O | 0.123 | 715 |
| C–N | 0.147 | 293 |
| C–Cl | 0.177 | 326 |
| C–F | 0.149 | 439 |
| O–H | 0.096 | 460 |
| N–H | 0.101 | 389 |
| Si–O | 0.164 | 368 |

A bond energy of 250 kJ/mol would correspond to a theoretical strength value of about $2.7 \cdot 10^4$ N/mm² after conversion. However, the effective strengths of unreinforced plastics are known to be much lower and are only between 10 N/mm² and 100 N/mm². This is a consequence of the weak points occurring in polymers, e. g., small voids as well as the weaker-acting secondary valence bonds between the macromolecules; see Section 2.1.4.2. Ultra-high-strength fibers with strengths of 3 to $5 \cdot 10^3$ N/mm² are an exception.

As far as the small voids are concerned, also referred to as *free volume*, they play a paramount role in the processing and existing properties of a plastic. Thus, the densification of a polymer by high pressures, i. e., the *decrease of the specific volume v* (in cm³/g) as a function of the pressure on the melt, is a central parameter in the primary molding and is detectable in the effects up to the use of a finished component; see Section 2.2.1.

Specific volume [cm³/g]

In contrast to the secondary valence bonds, the main valence bonds remain at their full strength during all thermoplastic processing, provided that no chemical reactions, e. g., oxidative-thermal damage, have occurred. Only when the decomposition temperature, $T_z$, is reached, the main valence bonds are destroyed; see Figure 2.6. This reveals another essential difference between low- and high-molecularweight materials: *the absence of a gas phase in macromolecules.* If, in addition, the macromolecules are chemically cross-linked with each other, as in the case of *elastomers and thermosets*, even the melt state can no longer be reached.

Absence of a gas phase