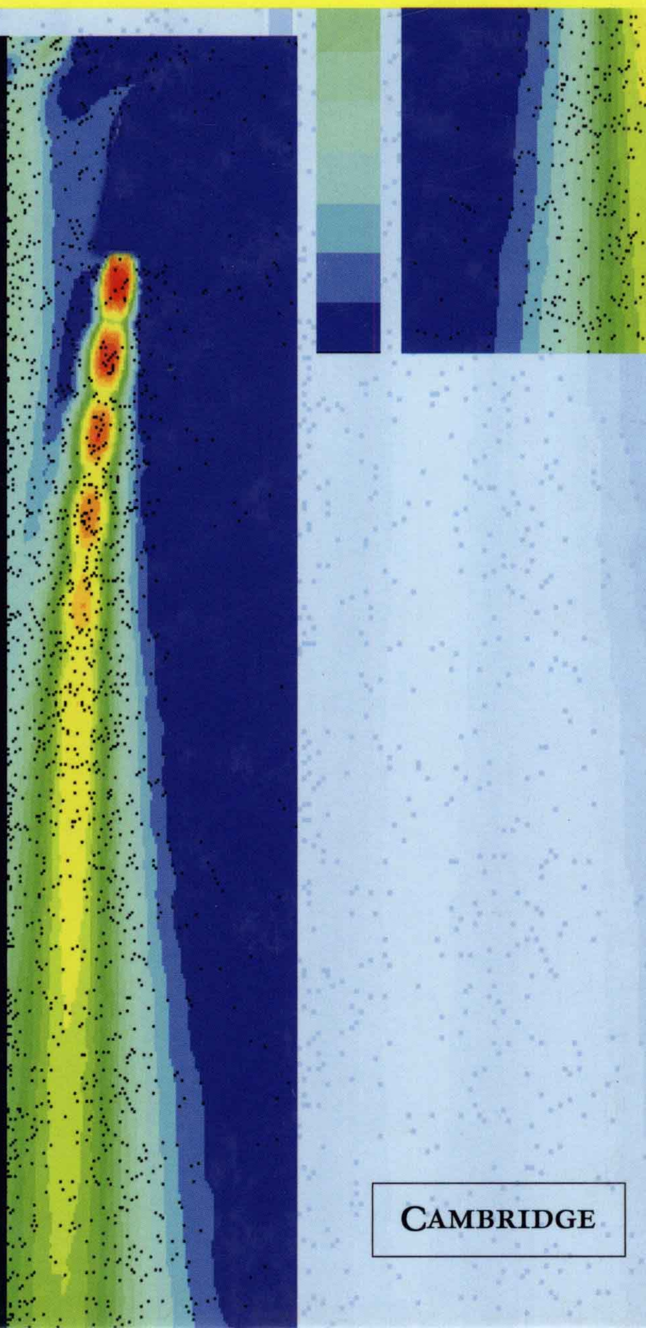
Spray Simulation

Modeling and Numerical Simulation of Sprayforming Metals

Udo Fritsching



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Preface

This book describes the fundamentals and potentials of modelling and simulation of complex engineering processes, based on, as an example, simulation of the spray forming process of metals. The spray forming process, in this context, is a typical example of a complex technical spray process. Spray forming, basically, is a metallurgical process whereby near-net shaped preforms with outstanding material properties may be produced direct from a metal melt via atomization and consolidation of droplets. For proper analysis of this process, first successive physical submodels are derived and are then implemented into an integrated coupled process model. The theoretical effects predicted by each submodel are then discussed and are compared to experimental findings, where available, and are summarized under the heading 'spray simulation'. The book should give engineering students and practising engineers in industry and universities a detailed introduction to this rapidly growing area of research and development.

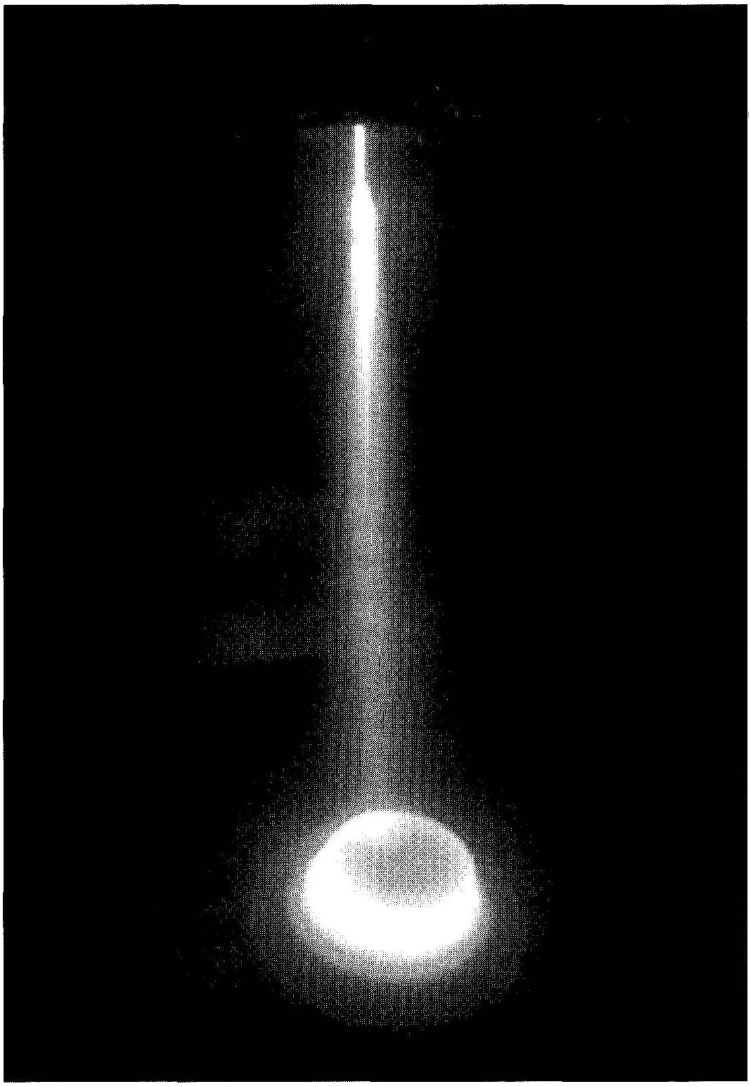
In order to develop an integral model for such technically complex processes as the spray forming of metals, it is essential that the model is broken down into a number of smaller steps. For spray forming, the key subprocesses are:

- atomization of the metal melt,
- dispersed multiphase flow in the spray,
- compaction of the spray and formation of the deposit.

These subprocesses may be further divided until a sequential (or parallel) series of unit operational tasks is derived. For these tasks, individual balances of momentum, heat and mass are to be performed to derive a fundamental model for each. In addition, some additional submodels need to be derived or applied. The general description of this modelling approach to the spray forming process is the fundamental aim of this book, which therefore:

- introduces a general modelling and simulation strategy for complex spray processes,
- reviews relevant technical contributions on spray form modelling and simulation, and
- analyses and discusses the physical behaviour of each subprocesses and materials in the spray forming process.

This work is based on a number of investigations of spray forming carried out by researchers all over the world. Major contributions have been given from research projects



conducted by the author's research group on 'multiphase flow, heat and mass transfer' at the University of Bremen, the Foundation Institute for Material Science (IWT), as well as the Special Research Cooperation Project on spray forming SFB 372 at the University of Bremen. These projects have been funded, for example, by the Deutsche Forschungsgemeinschaft DFG, whose support is gratefully acknowledged. Several graduate and PhD students contributed to this project. I would like to thank all of them for their valuable contributions, especially Dr.-Ing. O. Ahrens, Dr.-Ing. D. Bergmann, Dr.-Ing. I. Gillandt, Dr.-Ing. U. Heck, Dipl.-Ing. M. Krauss, Dipl.-Ing. S. Markus, Dipl.-Ing. O. Meyer and Dr.-Ing. H. Zhang. Also, I would like to thank those guests whom I had the pleasure of hosting at the University of Bremen and who contributed to the development of this book, namely Professor Dr.-Ing. C. T. Crowe and Professor Dr. C. Cui. I acknowledge Professor Dr.-Ing.

K. Bauckhage for initiating research in this field and thank him for his continuous support of research in spray forming at the University of Bremen.

I would like to thank my family, Karin and Anna, for their understanding and support.

In order to keep the price of this book affordable, it has been decided to reproduce all figures in black/white. All coloured plots and pictures can be found and downloaded by interested readers from the author's homepage. Some of the spray simulation programs used in this book may also be downloaded from this web page. The URL is:
www.iwt-bremen.de/vt/MPS/

Nomenclature

A	area	m^2
a_i	coefficients	
a	temperature conductivity	m^2/s
b_i	coefficients	
c_d	resistance (drag) coefficient	
c_p	specific heat capacity	kJ/kg K
c_1, c_2, c, c_T	constants of turbulence model	
D_k	dissipation	
d, D	diameter	m
$d_{3.2}$	Sauter mean diameter, SMD	m
d_{max}	maximum spread diameter	m
Ec	Eckart number	
F	force	N
F_f	volume ratio, filling function	
f_r	coefficient of friction, normalized resistance	
$f_{s,l}$	solid or liquid content	
f	frequency	1/s
f	distribution density of particles	
G	coefficient for interparticulate forces	
G	number of solid fragments	
g	gravity constant	m/s^2
$\dot{g}$	growth rate	m/s
GMR	mass flow rate ratio gas/metal	
H, h	height	m
H	enthalpy	kJ
h	specific enthalpy	kJ/kg
h_f	film thickness	m
h_l	ligament height	m
I, K	Bessel function	
J	nucleation rate	1/s
k_S	empirical constant	
k	turbulent kinetic energy	m^2/s^2
k_p	compaction rate	

k_B	Boltzmann constant	J/K
L	length	m
L_h	latent heat of fusion	kJ/kg
L_T	dissipation length scale	m
La	Laplace number	
l	length, distance to nozzle	m
M	fragmentation number	
$\dot{M}$	mass flow rate	kg/s
Ma	Mach number	
m	mass	kg
m	mode	
$\dot{m}$	mass flux	kg/m^2 s
Nu	Nusselt number	
N, n	number concentration, particle number	$1/m^3$
Oh	Ohnesorge number	
P	number of collisions	
Pe	Peclet number	
p	pressure	Pa
p	microporosity function	
q_r	probability density function	1/m
$\dot{Q}$	heat flow rate	W
$\dot{q}$	heat flux	W/m^2
r	radial coordinate	m
$r_{0.5}$	half-width radius	m
R	gas constant	kJ/kg K
R_L	Lagrangian time correlation coefficient	
Re	Reynolds number	
Real	real part	
S	source/sink	
Sha	Shannon entropy	
St	Stokes number	
Ste	Stefan number	
s	path	m
T	temperature	K
T^*	Stefan number	
$\dot{T}$	cooling rate (velocity)	K/s
ΔT	temperature difference	K
ΔT	undercooling	K
t	time	s
u, v, w	velocity components	m/s
V	volume	m^3
v	velocity of solidification front	m/s

W, **F**, **G**, **Q**	matrix	
We	Weber number	
x, y, z	plane Cartesian coordinates	m
x_K	length of supersonic core	m
x_s	mean distance between solid fragments	m
Z^*	splashing number	
z	distance atomizer – substrate	m
z, r, θ	cylindrical coordinates	m, m, °
α_G	gas nozzle inclination angle	°
α_f, α_g	volumetric content of gas, liquid	
α_{spray}	spray inclination angle	°
α	heat transfer coefficient	W/m^2 K
Γ	diffusivity	
Γ_S	Gamma function	
γ	solid–liquid surface tension	N/m
δ	excitation wavelength	m
δ	width of gas jets	m
ε	dissipation rate of turbulent kinetic energy	m^2/s^3
ε_S	radiation emissivity	
η_S	amplitude function of perturbation	
η_{ab}, η_B	amplitude of surface waves	
Θ_{col}	impact angle	°
θ	contact angle	°
θ	modified temperature	K
κ	isentropic exponent	
κ_0	surface curvature	1/m^2
λ	heat conductivity	W/m K
λ_0	reference heat conductivity	W/m K
λ_d	wavelength	m
λ_e	solidification coefficient	
μ	dynamic viscosity	kg/m s
ν	kinematic viscosity	m^2/s
ν_m	molar volume	m^3/mol
ξ_g	boundary layer coefficient	
ξ, η	dimensionless coordinates	
ρ	density	kg/m^3
σ_l	surface tension	N/m
σ_d	logarithmic standard deviation	
$\sigma_h, \sigma_{\frac{\varepsilon}{x}}, \sigma_k$	constants of turbulence model	
σ_S	Stefan–Boltzmann constant	W/m^2 K^4
σ_t	relative turbulence intensity	
τ	shear stress	N/m^2
τ_p	relaxation time	s

τ_T	eddy lifetime	s
τ_u	passing time through eddy	s
τ_v	interaction time	s
Φ	transport variable	
Φ	velocity potential	
Φ	impact angle	°
φ	velocity number	
χ	impact parameter	m
Ψ	stream function	
ψ_f	function of fluid density	
Ω	collision function	
ω	growth rate	1/s

Indices

A	nozzle exit area
a	lift
a	outer side
abs	total value
b	Basset
c	centre-line
c, crit	critical
ct	contact layer
cyl	cylindrical
d	dispersed phase (droplet)
eff	effective value
ener	energy
f	film
f	fluid
g	gas phase
g	gravity
h	hydrostatic
het	heterogeneous
hom	homogeneous
i	imaginary part
i	inner side
i, j	numbering, grid index
ideal	ideal state
in	inflow
jacket	side region of billet
k	nucleation
k	compaction
Lub	Lubanska
l	liquid

l	liquidus
m	mass
m	mean value
min, max	minimum value, maximum value
mom	moment
n	normal direction
out	melt exit
por	porosity
p	particle
p	pressure
p	projected
r	real part
rel	relative value
s	solidus
s	spray
Sh	shadow
sin	sinus
S	melt
t	turbulence
t	inertia
t	tangential direction
top	top side of billet
tor	torus
u	environment
v	velocity
w	wall
w	resistance
zu	addition
0	stagnation value
1	primary gas
2	secondary (atomization) gas
$*$	critical condition

Contents

1 Introduction

Modelling of technical production facilities, plants and processes is an integral part of engineering and process technology development, planning and construction. The successful implementation of modelling tools is strongly related to one's understanding of the physical processes involved. Most important in the context of chemical and process technologies are momentum, heat and mass transfer during production. Projection, or scaling, of the unit operations of a complex production plant or process, from laboratory-scale or pilot-plant-scale to production-scale, based on operational models (in connection with well-known scaling-up problems) as well as abstract planning models, is a traditional but important development tool in process technology and chemical engineering. In a proper modelling approach, important features and the complex coupled behaviour of engineering processes and plants may be simulated from process and safety aspects viewpoints, as well as from economic and ecologic aspects. Model applications, in addition, allow subdivision of complex processes into single steps and enable definition of their interfaces, as well as sequential investigation of the interaction between these processes in a complex plant. From here, realization conditions and optimization potentials of a complex process or facility may be evaluated and tested. These days, in addition to classical modelling methods, increased input from mathematical models and numerical simulations based on computer tools and programs is to be found in engineering practice. The increasing importance of these techniques is reflected by their incorporation into educational programmes at universities within mechanical and chemical engineering courses.

The importance of numerical models and simulation tools is increasing dramatically. The underlying physical models are based on several input sources, ranging from empirical models to conservation equations for momentum, heat and mass transport in the form of partial differential or integro differential equations. Substantial development of modelling and simulation methods has been observed recently in academic research and development, as well as within industrial construction and optimization of processes and techniques. For the process or chemical industries, some recent examples of the successful inclusion of modelling and simulation practice in research and development may be found, for example, in Birtigh *et al.* (2000). This increasing importance of numerical simulation tools is directly related to three different developments, which are individually important, as is the interaction between them:

- First, the potential of numerical calculation tools has increased due to the exploding power of the computer hardware currently available. Not only have individual single processor

computers increased their power by orders of magnitude in short time scales, but also interaction between multiple processors in parallel machines, computer clusters or vector computers has recently raised the hardware potential dramatically.
- Next, and equally important, the development of suitable sophisticated mathematical models for complex physical problems has grown tremendously. In the context of the processes to be described within this book, a variety of new complex mathematical models for the description of exchange and transport processes in single- and multiphase flows (based on experimental investigations or detailed simulations) has recently been derived.
- Last, but not least, developments in efficient numerical analysis tools and numeric mathematical methods for handling and solving the huge resulting system of equations have contributed to the increasing efficiency of simulated calculations.

Based on state-of-the-art modelling and simulation tools, a successful and realistic description of relevant technical and physical processes is possible. This story of success has increased the acceptance of numerical simulation tools in almost all technical disciplines. Closely connected to traditional and modern theoretical and experimental methods, numerical simulation has become a fundamental tool for the analysis and optimization of technical processes.

The process of spray forming, which will be discussed here in terms of modelling and simulation, is basically a metallurgical process, but will be mainly described from a fundamental process technology point of view. Metal spray forming and the production of metal powders by atomization, i.e. the technical processes evaluated in this book, are fundamentally related to the disintegration of a continuous molten metal stream into a dispersed system of droplets and particles. Atomization of melts and liquids is a classical process or chemical engineering operation, whereby a liquid continuum is transformed into a spray of dispersed droplets by intrinsic (e.g. potential) or extrinsic (e.g. kinetic) energy. The main purpose of technical atomization processes is the production of an increased liquid surface and phase boundary or interfacial area between liquid and gas. All transfer processes across phase boundaries directly depend on the exchange potential, which drives the process, and the size of the exchange surface. In a dispersed system, this gas/liquid contact area is equal to the total sum of surfaces of all individual drops, i.e. of all droplets within the spray. By increasing the relative size of the phase boundary in a dispersed system, the momentum, heat and mass transfer processes are intensified between the gas and the liquid. The total exchange flux within spray systems may thereby be increased by some orders of magnitude.

Atomization techniques in process technology or chemical engineering processes/plants can be applied to:

- impact-related processes, and
- spray-structure-related processes.

Some examples of spray process applications in engineering following this subdivision are listed below.

- Impact-related spray applications requiring a continuous fine spatial distribution of a liquid continuum, e.g. in the field of coating applications:

  - for protection of metallic surfaces from corrosion in mechanical engineering through paint application;
  - for coating of technical specimens/parts for use in private or industrial applications, including surface protection and colour (paint) application;
  - for thermal plasma- or flame-spraying of particles to provide protective ceramic or metallic coatings in the metal industry;
  - for spray granulation or coating of particles (for example in pelletizers or in fluidized beds), e.g. for pharmaceutical or food industry applications;
  - for spray cooling in steel manufacturing or in spray heat treatment of metallic specimens.
- Spray-structure-related applications whereby the structure or properties of liquids or particulate solids are altered by gas/dispersed phase exchange processes, within:
  - thermal exchange processes, e.g. for rapid cooling and solidification of fluid metal melts in metal powder generation;
  - coupled mass and thermal transfer processes, e.g. spray drying (or spray crystallization) in food or dairy industries or in chemical mass products production;
  - particle separation from exhaust gases, e.g. from conventional power plants (wet scrubbing);
  - reaction processes within fuel applications in energy conversion, automotive, or aeroplane or aerospace engine or fuel jet applications.
- Combination of impact- and spray-structure-related spray process applications:
  - within droplet-based manufacturing technologies, e.g. for rapid prototyping;
  - for the generation of specimens and preforms by spray forming of metals.

In spray forming, a combination of nearly all the features, subprocesses and examples of atomization processes listed, may be found. Spray forming is, in its unique composition, an ideal and typical example of a complex technical atomization process. The numerical modelling and simulation techniques derived for analysis and description of the spray forming process may be easily transferred to other atomization and spray process applications.

In a first analysis approach, the complex coupled technical process is subdivided into single steps for further study. In the context of spray forming, subdivision of the technical atomization process into modular subprocesses can be done. This is illustrated in Figure 1.1, where the three main subprocesses discussed below are shown:

- atomization: the process of fluid disintegration or fragmentation, starting with the continuous delivery of the fluid or melt, and necessary supporting materials (such as gases or additives), to the resulting spray structure and droplet spectrum from the atomization process;
- spray: the establishing and spreading of the spray, to be described by a dispersed multiphase flow process with momentum, heat and mass transfer in all phases, and the exchange between the phases, as well as a possible secondary disintegration process of fluid ligaments or coalescence of droplets;

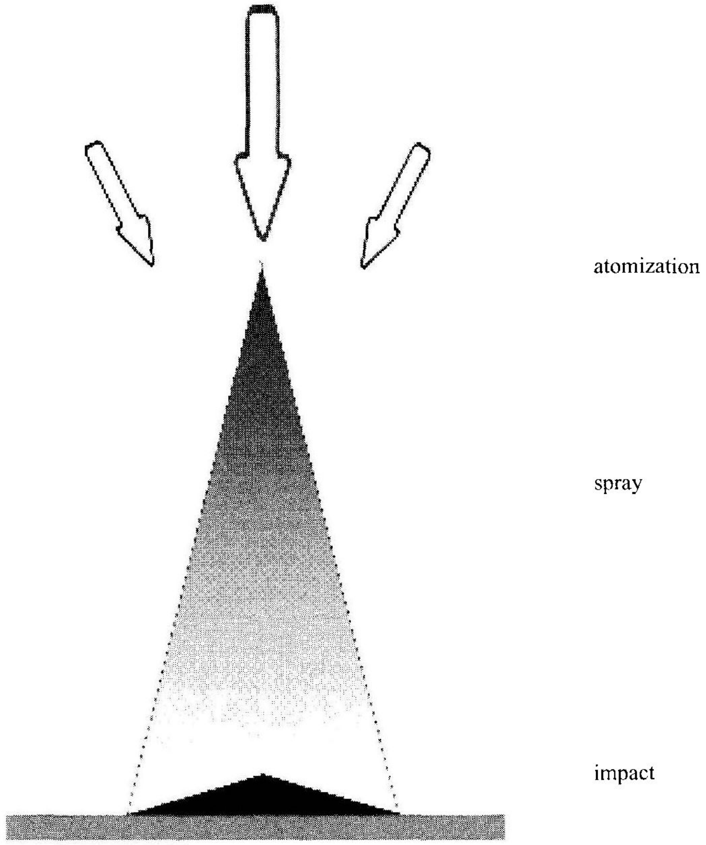


Fig. 1.1 Subdivision of an atomization process into subprocesses

- impact: the impact of spray droplets onto a solid or liquid surface and the compaction and growth of the impacting fluid or melt mass, as well as the building of the remaining layer or preform.

Central, integrative and common to all spray-related subprocesses is the fluids engineering and process or chemical engineering discipline of fluid dynamics in multiphase flows involving integral heat and mass transfer. The fundamental properties and applications of this discipline are central to the theme of this book.

Based on this method of analysis, modelling and numerical simulation are introduced as scientific tools for engineering process development, as applied to metal spray forming. Then, the individual physical processes that affect spray forming are introduced and implemented into an integral numerical model for spray forming as a whole. Recent modelling and simulation results for each subprocess involved during metal spray forming are discussed and summarized. Where possible, simulated results are compared to experimental results during spray forming, to promote physical understanding of the relevant subprocesses, and are discussed under the heading ‘spray simulation’.

Numerical modelling and simulation of the individual steps involved in spray forming are presently of interest to several research groups in universities and industry worldwide. In this book, the current status of this rapidly expanding research area will be documented. But despite the emphasis given to metal spray forming processes, it is a major concern of this book to describe common analysis tools and to explain general principles that the reader may then apply to other spray modelling strategies and to other complex atomization and spray processes.

To enhance the general integral spray forming model further, additional physical submodels need to be developed and boundary conditions determined. It is hoped that the combination of experimental, theoretical and numerical analyses presented here will contribute to the derivation and formulation of such additional subprocess models. Integration of these models into a general operational model of the spray forming process will then be possible.

In conclusion, the main aims of this book are:

- to introduce a general strategy for modelling and simulation of complex atomization and spray processes,
- to review relevant contributions on spray form modelling and simulation, and
- to analyse and discuss the physical behaviour of the spray forming process.