Development and Validation of a Numerical Model of the CO2 Dry-ice Blasting Process for Aircraft Engine Cleaning Applications

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Technological University Dublin

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Development and Validation of a Numerical Model of the CO₂ Dry-ice Blasting Process for Aircraft Engine Cleaning Applications

by


A thesis submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy (PhD) of the Dublin Institute of Technology

Volume 1/2

School of Mechanical and Design Engineering
Dublin Institute of Technology
May 2018

Dr. Barry Duignan
Dr. G. Reilly
Head of School

Prof. Dr.-Ing. Gerald Ruß
Supervisors
Abstract

On-wing cleaning of engine compressors for commercial aircraft is a required maintenance task which results in greater operating efficiency and lower emission rates. It is typically carried out by injection of water and detergents into the intake of an engine while the engine is being cranked by the starter. Two drawbacks of this process are the risk of icing in cold weather and the collection and treatment of the water effluent.

The dry-ice blasting process, a cleaning system which uses pressurized air and CO₂ dry-ice particles as cleaning agent, has been proposed as an alternative method which does not suffer the above drawbacks but is potentially capable of efficient cleaning. In this context, such a cleaning system is currently being developed by Lufthansa Technik in association with Hochschule Darmstadt and DIT. This work focuses on the development and validation of a numerical model of this process, which can be used to improve the understanding of the complex multiphase flow phenomena involved and to assess the cleaning physics.

Appropriate multiphase flow set-ups and new particle breakup and erosion models are developed. These new models will facilitate the numerical prediction of particle behaviour and defouling erosion rates during the defouling process.

An appropriate simulation set-up for the particle laden injection system flow simulations using the Euler-Lagrange method is investigated. Three possible injection systems with various air flow velocities and particle loading densities are considered. These systems are investigated by means of high-speed camera (HSC) experiments and the predicted results are compared to the experimental in order to find the best numerical set-up. An improvement to the particle drag force formulation is proposed for highly pressurized air-flows.

A new particle breakup model for dry-ice in Euler-Lagrange simulations is developed. This model is theoretically derived from an energy balance and un-
derpinned with data from HSC experiments. It includes velocity, impact angle and target temperature as factors determining breakup behaviour of dry-ice particles impinging solid walls.

A new defouling erosion model utilizing an energy balance approach and based on a range of experiments with several types of actual and artificial fouling material is developed and tested.

The particle breakup and the erosion model are implemented into the commercial CFD code Ansys CFX. Verification and validation studies of both new models are presented. The validation of the new models uses data acquired in a specially-designed wind-tunnel experiment.

All main findings and models are used in a final application case study where the new dry-ice based cleaning procedure is applied to a GE-CF6-50 test engine. Comparison of numerical results to data from air-flow, particle tracking and defouling experiments is also presented for this case.
Declaration

I certify that this thesis which I now submit for examination for the award of the degree of PhD, is entirely my own work and has not been taken from the work of others, save and to the extent that such work has been cited and acknowledged within the text of my work.

This thesis was prepared according to the regulations for graduate study by research of the Dublin Institute of Technology and has not been submitted in whole or in part for another award in any other third level institution. The work reported on in this thesis conforms to the principles and requirements of the DIT’s guidelines for ethics in research.

Signature __________________________________ Date _______________

PhD-Candidate Arthur Rudek

Darmstadt, 11. May 2018
Acknowledgements

I would like to thank my family, especially my wife Anja and my children Lian and Mika for their patience, support and encouragement during the recent four years. I know that this was a hard time for all of us.

I would like to acknowledge the contribution of my first supervisor, Prof. Dr.-Ing. Gerald Russ, without whose hard and time consuming preparation work this study would not have been possible. Furthermore, I would also like to acknowledge the contribution of my second supervisor, Dr. Barry Duignan, without whose patience this thesis would not be legible. Many thanks to both of you for your extensive discussions, for the permanent feedback and encouragement during the recent years.

I would also express my thanks to my HDA colleagues, especially to David Muckenhausen, Rudolf Kombeitz and Thomas-Alexander Zitzmann, to my Lufthansa Technik colleagues, especially to Dr.-Ing. Holger Appel, Dirk Deja, Ina Esemann and Stefan Kuntzagk, and also to all students and postgraduates who participated in parts of this study, for their kindness and help on many topics.

Finally, I would like to thank Prof. Dr.-Ing. Heinz-Peter Schiffer and Dr. Fergal Boyle for their time and their work on the final assessment of this thesis and Prof. Dr.-Ing. Peter Jeschke for the time he spent on the transfer report and for his valuable suggestions.

This work was carried out as research under the LuFo V programme, funded by the German BMWi and Lufthansa Technik as project Cyclean 2.0.
# Nomenclature

<table>
<thead>
<tr>
<th>UPPER-CASE Latin letters</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>m</td>
</tr>
<tr>
<td>OR parameter of potential function</td>
<td>OR $\frac{N}{m}$</td>
</tr>
<tr>
<td>AR</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>1</td>
</tr>
<tr>
<td>OR parameter of potential function</td>
<td>OR $\frac{N}{m}$</td>
</tr>
<tr>
<td>BU</td>
<td>1</td>
</tr>
<tr>
<td>C</td>
<td>various</td>
</tr>
<tr>
<td>D</td>
<td>m</td>
</tr>
<tr>
<td>diameter (i.e. of primary particle, bigger, outer etc.)</td>
<td></td>
</tr>
<tr>
<td>Df</td>
<td>1</td>
</tr>
<tr>
<td>E</td>
<td>J</td>
</tr>
<tr>
<td>OR erosion variable</td>
<td>OR various</td>
</tr>
<tr>
<td>ER</td>
<td>$\frac{mm^2}{mm}$</td>
</tr>
<tr>
<td>F</td>
<td>N</td>
</tr>
<tr>
<td>OR general function (specified by index)</td>
<td>OR various</td>
</tr>
<tr>
<td>Gr</td>
<td>1</td>
</tr>
<tr>
<td>H</td>
<td>$\frac{J}{m^3}$</td>
</tr>
<tr>
<td>I pixel intensity (i.e. relative to maximum intensity)</td>
<td>1</td>
</tr>
<tr>
<td>I intensity matrix</td>
<td>1</td>
</tr>
<tr>
<td>K</td>
<td>various</td>
</tr>
<tr>
<td>Kn</td>
<td>1</td>
</tr>
<tr>
<td>L length (i.e. maximum length of nozzle)</td>
<td>m</td>
</tr>
<tr>
<td>LHS left-hand side operator</td>
<td>various</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>M</td>
<td>mass (i.e. of large particle or total value)</td>
</tr>
<tr>
<td>Ma</td>
<td>Mach number</td>
</tr>
<tr>
<td>N</td>
<td>number (i.e. maximum count)</td>
</tr>
<tr>
<td>O</td>
<td>flowing contributors (i.e. to general governing equation)</td>
</tr>
<tr>
<td>P</td>
<td>productive contributors (i.e. to general governing equation)</td>
</tr>
<tr>
<td>Q</td>
<td>deviation assessment quotient</td>
</tr>
<tr>
<td>R</td>
<td>radius (i.e. bigger, outer)</td>
</tr>
<tr>
<td>Rs</td>
<td>specific gas constant</td>
</tr>
<tr>
<td>R²</td>
<td>coefficient of determination</td>
</tr>
<tr>
<td>Ra</td>
<td>roughness value (area averaged)</td>
</tr>
<tr>
<td>Ra</td>
<td>Rayleigh number</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>RHS</td>
<td>right-hand side operator</td>
</tr>
<tr>
<td>SNR</td>
<td>signal-to-noise ratio</td>
</tr>
<tr>
<td>St</td>
<td>Stokes number</td>
</tr>
<tr>
<td>T</td>
<td>temperature</td>
</tr>
<tr>
<td></td>
<td>OR total time</td>
</tr>
<tr>
<td>T</td>
<td>stress tensor</td>
</tr>
<tr>
<td>V</td>
<td>Volume</td>
</tr>
<tr>
<td>We</td>
<td>Weber number</td>
</tr>
<tr>
<td>Y</td>
<td>Youngs modulus</td>
</tr>
<tr>
<td>Z</td>
<td>feeding contributors (i.e. to general governing equation)</td>
</tr>
</tbody>
</table>

**lower-case Latin letters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>heat conductivity</td>
<td>(\frac{W}{mk})</td>
</tr>
<tr>
<td>OR speed of sound</td>
<td>OR (\frac{m}{s})</td>
<td></td>
</tr>
<tr>
<td>OR envelope velocity in x-direction</td>
<td>OR (m)</td>
<td></td>
</tr>
<tr>
<td>OR length scale</td>
<td>OR (m)</td>
<td></td>
</tr>
<tr>
<td>OR ellipse parameter (i.e. in erosion model)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
b  envelope velocity in y-direction  \(\frac{m}{s}\)  
OR length scale  \(m\)  
OR ellipse parameter (i.e. in erosion model)  

bu  breakup criterion (i.e. continuous)  1  

c  enveloppe velocity in z-direction  \(\frac{m}{s}\)  

c\(_D\)  drag coefficient  1  

c\(_p\)  specific heat capacity  \(\frac{J}{kg\cdot K}\)  

d  diameter  \(m\)  

dH  DeHaller criterion  1  

e  ambiguity criterion for particle tracking  \(m\)  
OR internal energy  \(\frac{J}{kg}\)  

ecc  elliptical eccentricity  1  

er  erosion rate (specific)  various  

f  general function (specified in context)  various  
OR focal distance (i.e. in erosion model)  \(m\)  

\(g\)  gravity  \(\frac{m}{s^2}\)  

h  specific enthalpy  \(\frac{J}{kg}\)  

k  turbulence kinetic energy  \(\frac{m^2}{s^2}\)  

\(k_B\)  Boltzmann constant  \(\frac{J}{K}\)  

\(k_r\)  roughness value  \(m\)  

m  mass  \(kg\)  
OR median value  \(\text{various}\)  
OR general exponent  \(\text{various}\)  

\(\dot{m}\)  mass flux  \(\frac{kg}{s}\)  

n  normal vector (i.e. in normal direction to a surface)  \(1\)  
OR general exponent  \(\text{various}\)  

\(\dot{n}_p\)  particle number rate  \(\frac{1}{s}\)  

o  flowing contributors in vector format (i.e. to general governing equation)  various  

p  pressure  \(Pa\)  
OR probability  \(1\)
productive contributors in vector format (i.e. to general governing equation)

heat-flux density $\frac{W}{m^2}$

radius (i.e. smaller) $m$

length scale $m$

source (general) various

time $s$

threshold value 1

velocity (i.e. fluid), direction specified by index $\frac{m}{s}$

velocity vector (i.e. fluid) $\frac{m}{s}$

velocity (i.e. solid particle), direction specified by index $\frac{m}{s}$

velocity vector (i.e. solid particle) $\frac{m}{s}$

spatial coordinate, direction specified by index $m$

spatial vector $m$

spatial coordinate, direction specified by system $m$

spatial coordinate, direction specified by system $m$

feeding contributors in vector format (i.e. to general governing equation) various

**UPPER-CASE Greek letters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma$</td>
<td>void fraction</td>
<td>1</td>
</tr>
<tr>
<td>$\Theta$</td>
<td>angle (i.e. shock)</td>
<td>$deg$</td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>general assessment variable</td>
<td>various</td>
</tr>
<tr>
<td></td>
<td>(i.e. for deviations etc.)</td>
<td></td>
</tr>
<tr>
<td>$\Upsilon$</td>
<td>dimensionless coefficient</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>(i.e. specified by index)</td>
<td></td>
</tr>
<tr>
<td>$\Phi$</td>
<td>general transport variable (vector format)</td>
<td>various</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>potential function</td>
<td>$\frac{N}{m}$</td>
</tr>
<tr>
<td>lower-case Greek letters</td>
<td>Unit</td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>-------------------</td>
<td></td>
</tr>
<tr>
<td>( \alpha )</td>
<td>angle (i.e. impact angle) ( \text{deg} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR particle area   ( \text{m}^2 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR breakup parameter ( \text{m}^{\frac{3}{2}} )</td>
<td></td>
</tr>
<tr>
<td>( \beta )</td>
<td>breakup parameter</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR thermal expansion coefficient ( \frac{m}{\text{s}^2} )</td>
<td></td>
</tr>
<tr>
<td>( \gamma )</td>
<td>flow or particle direction (i.e. angle) ( \text{deg} )</td>
<td></td>
</tr>
<tr>
<td>( \gamma_0 )</td>
<td>internal (bond) energy ( \frac{J}{m^2} )</td>
<td></td>
</tr>
<tr>
<td>( \delta )</td>
<td>symbol used for differences (any) various</td>
<td></td>
</tr>
<tr>
<td>( \delta h )</td>
<td>heat of fusion (phase change enthalpy) ( \frac{J}{\text{kg}} )</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>coefficient of restitution 1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR pixel energy measure (tracking) ( \frac{m^2}{\text{s}^3} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR turbulence eddy dissipation</td>
<td></td>
</tr>
<tr>
<td>( \varepsilon_r )</td>
<td>equivalent roughness value 1</td>
<td></td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>theoretical sublimation rate 1</td>
<td></td>
</tr>
<tr>
<td>( \zeta )</td>
<td>position variable (any) various</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR loss coefficient (in pressure loss formulation)</td>
<td></td>
</tr>
<tr>
<td>( \eta )</td>
<td>diffusion coefficient (i.e. dynamic viscosity) various</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR efficiency (i.e. compressor)</td>
<td></td>
</tr>
<tr>
<td>( \theta )</td>
<td>mass moment of inertia ( \text{kg} \cdot \text{m}^2 )</td>
<td></td>
</tr>
<tr>
<td>( \kappa )</td>
<td>isentropic exponent 1</td>
<td></td>
</tr>
<tr>
<td>( \lambda )</td>
<td>heat conductivity ( \frac{W}{m \cdot K} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR numerical particle number loading</td>
<td></td>
</tr>
<tr>
<td>( \lambda^* )</td>
<td>molecular length scale ( m )</td>
<td></td>
</tr>
<tr>
<td>( \mu )</td>
<td>thickness (i.e. fouling layer) ( m )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR mean value (i.e. statistical approach) various</td>
<td></td>
</tr>
<tr>
<td>( \nu )</td>
<td>kinematic viscosity ( \frac{m^2}{\text{s}} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR Poison ratio ( \frac{m^2}{\text{s}} )</td>
<td></td>
</tr>
<tr>
<td>( \xi )</td>
<td>random variable (i.e. specified by index) 1</td>
<td></td>
</tr>
<tr>
<td>( \pi )</td>
<td>natural constant 1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>OR pressure ratio 1</td>
<td></td>
</tr>
</tbody>
</table>
\( \rho \) density \( \frac{kg}{m^3} \)

\( \sigma \) standard deviation

OR superficial energy \( \frac{J}{m} \)

\( \tau \) specific time \( s \)

OR temperature ratio OR 1

\( \phi \) general transport variable various

\( \chi \) general pdf-variable various

\( \psi \) vector symbol for various material properties various

\( \omega \) rotational speed \( \frac{1}{s} \)

OR turbulent eddy frequency

OR frequency (in frequency domain)

**Indexes**

<table>
<thead>
<tr>
<th>Index</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>initial ( OR ) constant order</td>
</tr>
<tr>
<td>0°</td>
<td>variable at normal impact ( i.e. in defouling erosion model )</td>
</tr>
<tr>
<td>1</td>
<td>first</td>
</tr>
<tr>
<td>2</td>
<td>second</td>
</tr>
<tr>
<td>99</td>
<td>end of boundary layer ( i.e. ) thickness definition</td>
</tr>
<tr>
<td>+</td>
<td>upper or positive ( i.e. ) direction ( OR ) non-dimensional ( i.e. ) wall function</td>
</tr>
<tr>
<td>-</td>
<td>lower or negative ( i.e. ) direction</td>
</tr>
<tr>
<td>*</td>
<td>characteristic value ( OR ) modified value</td>
</tr>
<tr>
<td>( \infty )</td>
<td>infinite ( OR ) ambience</td>
</tr>
<tr>
<td>ADD</td>
<td>additional</td>
</tr>
<tr>
<td>air</td>
<td>related to air</td>
</tr>
<tr>
<td>amb</td>
<td>ambient</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>angle ( i.e. ) parameter in defouling erosion model</td>
</tr>
<tr>
<td>BG</td>
<td>background</td>
</tr>
<tr>
<td>BY</td>
<td>related to the bypass ( i.e. ) of the engine</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------</td>
</tr>
<tr>
<td>bb</td>
<td>bounding box</td>
</tr>
<tr>
<td>bu, BU</td>
<td>breakup</td>
</tr>
<tr>
<td>c</td>
<td>classes (i.e. particle size, velocity etc.)</td>
</tr>
<tr>
<td>cfx</td>
<td>Ansys CFX (i.e. the particle breakup and erosion model implementation)</td>
</tr>
<tr>
<td>cont</td>
<td>continuous phase</td>
</tr>
<tr>
<td>conv</td>
<td>convergent</td>
</tr>
<tr>
<td>cor</td>
<td>correlation</td>
</tr>
<tr>
<td>corr</td>
<td>corrective</td>
</tr>
<tr>
<td>CO₂</td>
<td>related to carbon-dioxide</td>
</tr>
<tr>
<td>CLASS</td>
<td>related to any class (i.e. particle size class)</td>
</tr>
<tr>
<td>d</td>
<td>diameter (i.e. of secondary particles)</td>
</tr>
<tr>
<td>deb, DEB</td>
<td>debris (i.e. particle size class)</td>
</tr>
<tr>
<td>diff</td>
<td>describing a difference (i.e. in a matrix)</td>
</tr>
<tr>
<td>dir</td>
<td>direction (any)</td>
</tr>
<tr>
<td>disp</td>
<td>dispersed phase (i.e. particles)</td>
</tr>
<tr>
<td>diss</td>
<td>dissipative</td>
</tr>
<tr>
<td>div</td>
<td>divergent</td>
</tr>
<tr>
<td>dp</td>
<td>pressure gradient (i.e. force)</td>
</tr>
<tr>
<td>drag</td>
<td>drag (i.e. force)</td>
</tr>
<tr>
<td>dust</td>
<td>dust (i.e. particle size class)</td>
</tr>
<tr>
<td>ecc</td>
<td>eccentricity</td>
</tr>
<tr>
<td>ell</td>
<td>elliptical</td>
</tr>
<tr>
<td>er</td>
<td>erosive</td>
</tr>
<tr>
<td>erm</td>
<td>erosion model (any)</td>
</tr>
<tr>
<td>err</td>
<td>error</td>
</tr>
<tr>
<td>exp</td>
<td>experimental</td>
</tr>
<tr>
<td>EQ</td>
<td>equivalent (i.e. velocity value)</td>
</tr>
<tr>
<td>ε</td>
<td>related to turbulent dissipation rate</td>
</tr>
<tr>
<td>F</td>
<td>related to fluid</td>
</tr>
<tr>
<td>fou</td>
<td>fouling</td>
</tr>
<tr>
<td>GEN</td>
<td>particle generation history (i.e. particle breakup model)</td>
</tr>
</tbody>
</table>
\( \eta \) related to viscous contribution (i.e. turbulence model)

hda Hochschule Darmstadt

(i.e. the particle breakup and erosion model implementation)

imp, related to impact (i.e. angle, velocity, area etc.)

IMP

I intensity

in, IN related to inlet

i, j counting index OR direction index

i \rightarrow j from i to j (i.e. range of random variable)

I, II first and second (i.e. pole in histogram)

k related to turbulent kinetic energy

kb Boltzmann constant

kin kinetic (i.e. energy)

L large (particles)

m, n upper counting bounds

man manufacturing

mx maximum

MAX maximum

MIN minimum

n normal (i.e. direction)

OR number (i.e. of secondary particles)

node related to nodal area of influence (FEM)

num numerical

N total number (counting bound)

ORIG1 original fouling material from lower compressor stages (i.e. with significant amounts of carbon)

ORIG2 original fouling material from higher compressor stages (i.e. no significant amounts of carbon)

OP opening (i.e. boundary condition)

out related to an outlet (i.e. engine, wind-tunnel experiment, nozzle etc.)

\( \omega \) related to turbulent eddy frequency
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>p</td>
<td>production</td>
</tr>
<tr>
<td>part</td>
<td>related to particle material (i.e. dry-ice in defouling action)</td>
</tr>
<tr>
<td>pc</td>
<td>phase change</td>
</tr>
<tr>
<td>post</td>
<td>post (after) impact</td>
</tr>
<tr>
<td>pot</td>
<td>potential (i.e. energy)</td>
</tr>
<tr>
<td>pre</td>
<td>pre (before) impact</td>
</tr>
<tr>
<td>proj</td>
<td>projected (i.e. area)</td>
</tr>
<tr>
<td>ps</td>
<td>pressure side</td>
</tr>
<tr>
<td>P</td>
<td>particle related</td>
</tr>
<tr>
<td>PTFE</td>
<td>Polytetrafluoroethylene (i.e. artificial fouling material)</td>
</tr>
<tr>
<td>φ</td>
<td>related to any physical variable</td>
</tr>
<tr>
<td>r</td>
<td>roughness related</td>
</tr>
<tr>
<td>red</td>
<td>reduced (i.e. mass-flux)</td>
</tr>
<tr>
<td>ref</td>
<td>related to reference (i.e. material)</td>
</tr>
<tr>
<td>res,</td>
<td>residual (i.e. particle size class)</td>
</tr>
<tr>
<td>RES</td>
<td></td>
</tr>
<tr>
<td>rot</td>
<td>rotatoric (i.e. energy, system etc.)</td>
</tr>
<tr>
<td>R</td>
<td>Reynolds Stress Tensor</td>
</tr>
<tr>
<td>s</td>
<td>setting (any)</td>
</tr>
<tr>
<td>OR isentropic (i.e. efficiency)</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>small (particles)</td>
</tr>
<tr>
<td>OR ideal gas (i.e. constant)</td>
<td></td>
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<tr>
<td>sek,</td>
<td>secondary (i.e. particles after impact)</td>
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<tr>
<td>SEK</td>
<td></td>
</tr>
<tr>
<td>ss</td>
<td>suction side</td>
</tr>
<tr>
<td>stat</td>
<td>stationary (i.e. system)</td>
</tr>
<tr>
<td>sub</td>
<td>sublimation</td>
</tr>
<tr>
<td>SALT</td>
<td>salt layer (i.e. artificial fouling material)</td>
</tr>
<tr>
<td>t</td>
<td>time related (i.e. certain instant of time)</td>
</tr>
<tr>
<td>OR total (i.e. pressure, temperature etc.)</td>
<td></td>
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<tr>
<td>tar</td>
<td>target</td>
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<tr>
<td>th</td>
<td>thermal</td>
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</tbody>
</table>
tot, total
TOT
trans translatic
trv threshold value
turb turbulent
x, y, z direction indicators

Special mathematical symbols

\( \mathcal{F} \) filter function (i.e. in FFT-based filtering)
\( \Theta \) order of magnitude
\( \Re \) residual
\( \mathrm{sig} \) signum function
\( := \) definition
\( \dagger \) constraint
\( \lceil \rceil \) rounding indicator

Abbreviations

2D, 3D two dimensional, three dimensional
Al aluminium
AMB ambience, ambient
B blade (i.e. rotor of the compressor)
BLMH bellmouth
BU breakup
CFD computational fluid dynamics
dimls dimensionless
DEM discrete element method
DI dynamic indentation (i.e. testing)
DIT Dublin Institute of Technology
DNS direct numerical simulation
EGT exhaust gas temperature
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EXP, exp</td>
<td>experimental</td>
<td></td>
</tr>
<tr>
<td>et al.</td>
<td>et aliae</td>
<td></td>
</tr>
<tr>
<td>etc</td>
<td>et cetera</td>
<td></td>
</tr>
<tr>
<td>FEM</td>
<td>finite element method</td>
<td></td>
</tr>
<tr>
<td>FVM</td>
<td>finite volume method</td>
<td></td>
</tr>
<tr>
<td>GE</td>
<td>General Electric (company)</td>
<td></td>
</tr>
<tr>
<td>hda,</td>
<td>Hochschule Darmstadt, University of Applied Sciences</td>
<td></td>
</tr>
<tr>
<td>HDA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HPC</td>
<td>high-pressure compressor</td>
<td></td>
</tr>
<tr>
<td>HSC</td>
<td>high speed camera</td>
<td></td>
</tr>
<tr>
<td>i.e.</td>
<td>id est</td>
<td></td>
</tr>
<tr>
<td>IBM</td>
<td>immersed boundary method</td>
<td></td>
</tr>
<tr>
<td>IMG</td>
<td>image</td>
<td></td>
</tr>
<tr>
<td>IGV</td>
<td>inlet guide vane</td>
<td></td>
</tr>
<tr>
<td>LDV</td>
<td>laser doppler velocimetry</td>
<td></td>
</tr>
<tr>
<td>LHS</td>
<td>left hand side</td>
<td></td>
</tr>
<tr>
<td>LHT</td>
<td>Lufthansa Technik AG</td>
<td></td>
</tr>
<tr>
<td>LPC</td>
<td>low-pressure compressor</td>
<td></td>
</tr>
<tr>
<td>MV</td>
<td>mechanical velocimeter</td>
<td></td>
</tr>
<tr>
<td>NUM,</td>
<td>numerical</td>
<td></td>
</tr>
<tr>
<td>num</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OGV</td>
<td>outlet guide vane</td>
<td></td>
</tr>
<tr>
<td>ORIG1</td>
<td>original fouling material from lower compressor stages (i.e. with significant amounts of carbon)</td>
<td></td>
</tr>
<tr>
<td>ORIG2</td>
<td>original fouling material from higher compressor stages (i.e. no significant amounts of carbon)</td>
<td></td>
</tr>
<tr>
<td>PIV</td>
<td>particle image velocimetry</td>
<td></td>
</tr>
<tr>
<td>PTFE</td>
<td>Polytetrafluoroethylene (i.e. artificial fouling material)</td>
<td></td>
</tr>
<tr>
<td>PTV</td>
<td>particle tracking velocimetry</td>
<td></td>
</tr>
<tr>
<td>POM</td>
<td>polyethylmexylene</td>
<td></td>
</tr>
<tr>
<td>POST</td>
<td>post or after (i.e. impact)</td>
<td></td>
</tr>
<tr>
<td>PRE</td>
<td>pre or before (i.e. impact)</td>
<td></td>
</tr>
<tr>
<td>RHS</td>
<td>right hand side</td>
<td></td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
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<td>--------------</td>
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<td></td>
</tr>
<tr>
<td>SALT</td>
<td>salt layer (i.e. artificial fouling material)</td>
<td></td>
</tr>
<tr>
<td>TBC</td>
<td>thermal barrier coating</td>
<td></td>
</tr>
<tr>
<td>TOW</td>
<td>time on wing</td>
<td></td>
</tr>
<tr>
<td>TRY</td>
<td>theoretical (i.e. analysis)</td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>vane (i.e. stator of the compressor)</td>
<td></td>
</tr>
<tr>
<td>WC</td>
<td>tungsten carbide</td>
<td></td>
</tr>
</tbody>
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1 Introduction

This Chapter comprises an introduction to on-wing axial aircraft compressor cleaning which is the application case for all research results presented in this study. The background and the motivation for this work are described in section 1.1. The main benefits of regular aircraft engine compressor cleaning are highlighted and a brief introduction of currently-used cleaning systems is given. In section 1.2 the topic of research is defined and the academic void which is addressed by this work is highlighted. Finally, the contribution of this work to progress in the current field of research is outlined.

1.1 Background and motivation

On-wing compressor cleaning systems are used by commercial aircraft operators to improve aircraft engine performance, which enhances the operator's competitiveness. Engine maintenance cost represents approximately 35 % to 40 % of an airline's total maintenance cost due to ACKERT [1]. Axial aircraft compressor fouling causes a range of negative effects on engine performance. An increase of airfoil roughness and fouling layer thickness leads to decreasing pressure and temperature ratio, decreasing core mass flux and hence a decrease of the surge and stall margin and of the efficiency of the compressor (i.e. component efficiency and pressure ratio), which represents approximately 70 % of an engine's total thermal efficiency [44, 114, 116, 117, 118, 131, 139]. To maintain constant thrust when engines are fouled, more fuel must be burned during operation. This leads to higher fuel consumption, higher emission rates and higher exhaust gas temperatures (EGT). An increased EGT deteriorates the hot path of the engine. Combustion chambers as well as the turbines face higher stresses. Corrosion of compressor blades is also possible.

Cleaning systems such as the currently-used water-wash system are applied directly to the on-wing engine during aircraft ground time. In order to wash
Figure 1.1.: Current water-wash systems, LHT Cyclean (left) [112] and P&W Ecopower (right) [154].

the engine, an air flow, which is laden with solid or liquid detergents, is injected into the dry-cranked engine. Two examples for such systems are presented in Fig. 1.1. The left-hand image shows Lufthansa Technik’s (LHT) Cyclean system and the right-hand image shows Pratt & Whitney’s (P&W) Ecopower system. In both cases heated water droplets are injected into the engine core, which is shown schematically in Fig. 1.2 and discussed below. While the Cyclean system is directly mounted to the engine’s fan and rotates with the dry-cranked engine, the Ecopower system is mounted stationary in front of the rotating fan blades. Fuel savings in the range from 1.0 % [112] to 1.2 % [154] and lower EGTs up to a decrease of 15°C [112, 154] are possible if engines are regularly washed.

Figure 1.2.: Schematic of aircraft compressor cleaning, here shown for dry-ice.
The general procedure is shown schematically in Fig. 1.2 using the case of CO$_2$ dry-ice cleaning. Compressor blades are defouled by particle-wall (or droplet-wall) interaction. A range of mechanisms can cause defouling, which are mainly dependent on the combination of detergent (particles or droplets) and fouling material [28]. But the most important defouling mechanism is not sensitive to the detergent used and it is the mechanical effect, which is caused by the kinetic energy of impacting particles or droplets [28, 130, 131]. However, there are also detergent and fouling dependent mechanisms to be considered (i.e. non-mechanical), such as dissociation-driven defouling of salt layers by water droplets.

The deterioration factors discussed above lead to earlier maintenance-shop visits and decrease in the number of flight cycles of the engines. The decision for a shop visit is mainly influenced by the critical EGT margin [1]. Figure 1.3 illustrates this using a dataset from ACKERT [1]. The figure compares the EGT margin of an aircraft engine as a function of the number of flight cycles (here both dimensionless) for a non-cleaned engine and a regularly cleaned engine. The number of flight cycles and the available EGT margin increase for a certain number of flight cycles with regular on-wing compressor cleaning (here water-wash). The operator saves fuel and maintenance cost and the life-cycle of the engine increases. Comparable data is presented for industrial gas turbines for example in [76].

![Figure 1.3](image-url)

**Figure 1.3.** EGT margin vs. No. of Flight Cycles for regularly water-washed and non-cleaned engine; dataset from ACKERT [1].
The engine cleaning procedure is still a topic of research for LHT, since the existing Cyclean system has two main disadvantages. The first is the legal requirement to collect and dispose waste water, which makes the cleaning process lengthy and expensive. Secondly, the threat of icing inside engines makes water based systems usable down to ambient temperatures as low as 7°C, which limits the applicability of the system to warmer regions of the world or to certain periods of the year only. To overcome these disadvantages, LHT is currently developing a CO₂ dry-ice based cleaning system in cooperation with Hochschule Darmstadt, University of Applied Sciences, (hda) and Dublin Institute of Technology (DIT).

Since CO₂ dry-ice sublimes directly at ambient conditions (i.e. $p_{amb} = 1.013 \text{ bar}$ and $T_{amb} = 20^\circ\text{C}$), there is no cleaning residue to be disposed. The danger of icing is removed since there is no humidity inside of the engine during the cleaning-process. The global CO₂ balance is not negatively influenced by the process, because the dry-ice used is a by-product from the chemical industry [198]. Furthermore, a higher efficiency of dry-ice based defouling is expected compared to water-based cleaning, since the mechanical defouling effect increases due to higher density and hardness of dry-ice compared to water droplets.

The key goal of this current development project is to numerically simulate the dry-ice based defouling process of axial aircraft compressor sections. It is planned to achieve this advance of the current state of the art of engine defouling predictions by means of a new and validated simulation procedure, which incorporates the development of new models for dry-ice particle breakup and defouling erosion. Such simulations help to deeper understand the process during the development phase. Furthermore, it is desired to use these simulations instead of expensive and time consuming experiments for process dimensioning and generalization, and for the optimization of process parameters.

### 1.2 Topic of research

The main focus of this work is the physical understanding of CO₂ dry-ice laden multiphase flow systems, which are used for cleaning purposes in axial com-
pressors of commercial aircraft engines. An appropriate multiphase-flow simulation strategy, a particle breakup model and an erosion model for the numerical prediction of detailed flow and cleaning patterns are therefore developed.

Typical particle laden cleaning flows, fouling materials and geometries are considered. The models are used with CFD simulations using Ansys CFX. The final goal of this work is the reliable numerical prediction of defouling erosion (here airfoil defouling), which can be used to understand and optimize various cleaning-system parameters.

The study presented is split into three main sections: dealing with the investigations of dry-ice injection systems, the development of a dry-ice particle breakup model for Euler-Lagrange simulations and the development of a defouling erosion model for dry-ice. The following section provides a brief introduction to each of these topics and highlights the academic voids addressed. Chapter 2 contains a detailed theoretical introduction to the systems investigated and Chapter 3 contains a detailed state-of-the-art survey for each of the research topics introduced here.

1.2.1 Dry-ice injection systems

Dry-ice wash flows are introduced into aircraft engines by means of conventional dry-ice blasting machines and this is for example described in [59]. Particles are accelerated by means of compressed air through convergent or convergent-divergent nozzles. The accelerating flow regime is usually compressible and can be subsonic, transonic or supersonic, depending on the machine settings. This air flow is discontinuously laden with dispersed particles of various shape and size. Particle size, assumed to be represented by the diameter of an ideal sphere in this work, varies from several $\mu$m up to a few mm. Comparable cases of particle transportation can be found in a number of industrial sectors such as cleaning, chemical, power, food, materials etc.

Examples of numerical investigations of particle laden compressible flows can be summarized as follows: simulations of conventional dry-ice blasting were utilized in thermal spray development studies by DONG et al. [48] who used
Ansys FLUENT. The prediction of dissociation and distribution processes of dispersed particles (in this case water droplets) in supersonic injector systems was investigated numerically by ADAMOPOULOS and PETROPAKIS [2] with FLUENT/UNS. An application case from the chemical industry is gas-assisted atomization, which was described and investigated by means of an Euler-Euler approach by POUGATCH et al. [152], who utilized code from the Netlib depository. In cold spraying applications, solid particles are accelerated by means of convergent-divergent nozzle systems and this was investigated numerically for example by YIN et al. [209] with Ansys FLUENT. However, the initial literature review revealed a lack of experimental data and numerical set-up validation studies for flow regimes in conjunction with particles and geometries such as these described here. For this reason, novel experiments and simulations are addressed in this work in section 3.2 and Chapter 4.

1.2.2 Particle breakup modelling

Currently, there are no features implemented in Ansys CFX for solid particle breakup predictions in Euler-Lagrange large scale simulations. One possibility to calculate particle breakup using this code is to diversify existing secondary droplet breakup models, such as those described by O’ROURKE and AMSDEN [140] or TANNER [190]. This approach requires appropriate calibration and abstraction of physical properties, because those models were originally developed and validated for gas-fluid induced interaction effects. However, it is not possible to cover the real physics of solid dry-ice particle breakup by abstraction of the above models (for details see section 3.3 and Chapter 5).

In small scale simulations, in contrast, it is possible to calculate solid particle breakup processes. This breakup is induced by the interaction of particles (in these cases granules) with their ambient environment. The associated simulation method is discrete element modelling (DEM), which was used by many research groups, for example THRONTON et al. [96, 125, 193] or ANTONYUK et al. [10, 11, 12]. However, DEM modelling cannot be used for the application case at hand, because it is a small scale methodology, which requires the modelling of each global agglomerate consisting of thousands of primary particles.
For each of these, a set of equations of motion must be solved [11]. This and the
necessity to simulate particle motion coupled with airflow through the machine
(in this case axial aircraft compressors) makes it numerically impossible to map
a large scale commercial aircraft engine compressor defouling simulation using
DEM in a computationally affordable manner.

Furthermore, there is no exact information published to date dealing with
the particle breakup behaviour of dry-ice particles. For the above reasons,
an experimentally-based particle breakup model for Euler-Lagrange dry-ice de-
fouling simulations is presented in this study in Chapter 5. The experimental
database is used to discuss general dry-ice particle impact and disintegration
behaviour. The model is eventually used in a validation case study present-
ted in Chapter 7 and in aircraft engine defouling simulations with Ansys CFX
presented in Chapter 8.

### 1.2.3 Defouling erosion modelling

In commercial CFD codes there are usually empirical or semi-empirical mod-
els for erosion prediction included. These models consist of algebraic formu-
lations, which account for a certain number of flow properties and substrate
materials (for example sand laden air flow in stainless steel pipes). Examples
of various approaches are given in [161]. An example of an empirical model
is from SALAMA (description from BARTON [19]), which is applicable to di-
lute gas-particle multiphase flows in channels in Euler-Euler simulations. Semi-
empirical models, such as the direct impingement model (DIM) developed by
CHEN et al. [39] and ZHANG et al. [214] or the model presented by OKA et
al. [137, 138], predict erosion in a more general way and usually account for
particle impact velocity and impact angle.

The macro scale dynamic model (MSDM) presented by LI at al. [37, 108] is
based on a macroscopic spatial discretization and modelling of target mater-
ial. It consists of mass-points linked via a grid structure representing material
properties and is typically used for crystalline or compound materials. Models
such as these by CHEN [39] and OKA [137, 138] could possibly be used for the
current application case after an appropriate calibration study.
Ansys CFX however incorporates the turbomachinery-specific erosion models from FINNIE [56] and GRANT and TABAKOFF [67]. FINNIE [56] analysed the basic principles of ductile and solid target material erosion and gave basic relations between erosion rate, particle impact velocity and impact angle. GRANT and TABAKOFF [67] developed a full theoretical approach to predict particle trajectories and rebounding behaviour as well as erosive action of particles investigated in turbomachinery. However, neither of the above models was designed to predict airfoil defouling by means of dry-ice particles. Hence, an experimentally-based erosion model is presented in Chapter 6. It comprises a range of fouling materials typically found on aircraft compressor airfoils and it describes the defouling action of impinging dry-ice particles. The model is also used in the validation case study presented in Chapter 7 and in the final aircraft engine defouling simulations presented in Chapter 8.

1.2.4 Summary of the contribution of this work

Taking into account the academic voids identified above, this work provides a theoretical investigation and various experiments and numerical simulations with Ansys CFX for an experimentally underpinned and validated strategy to numerically predict erosive airfoil defouling of commercial aircraft engine compressors with dry-ice. The final simulation procedure is usable in an industrial environment.

The assessment and enhancement of the predictive capabilities of the Ansys CFX toolbox is addressed in terms of particle trajectory predictions in conjunction with complex flows. Dispersed particle interaction with solid walls is discussed in terms of extensive experimental particle breakup studies, from which a new particle breakup model is derived. Numerous experiments are also presented to assess erosion rates of a range of fouling materials which can typically be found on compressor airfoils. With this data, the influence of fouling upon particle breakup is discussed and a new defouling erosion model is created.

In summary, the main objectives of this work (all related to simulations with Ansys CFX) are:
• assessment of the predictive capabilities of the Lagrangian particle transport toolbox

• determination of the best set-up for Euler-Lagrangian dry-ice laden particle transport simulations

• extension of the Lagrangian particle transport toolbox with a dry-ice particle breakup model

• extension of the erosion toolbox with a defouling erosion model

• verification and validation of all above developments using experimental and numerical work

• utilization of the above findings, modifications and models in an application case simulation

The particle-breakup model for dry-ice and the defouling erosion model for various dry-ice and fouling combinations are identified as new technologies developed and presented in this study. Furthermore, numerical Euler-Lagrangian particle tracking and experimental HSC based particle tracking velocimetry (PTV) are existing technologies applied in a novel context, which is:

• examination and validation of a number of typical dry-ice injection system flows using substitute and dry-ice particles

• detailed examination of the particle laden flow from a novel re-engineered transparent supersonic dry-ice blasting nozzle

• detailed investigation of particle laden flows inside a novel transparent wind-tunnel experiment and inside a real aircraft engine compressor

• execution of basic single-particle experiments for the development of a statistical database to the novel particle-breakup and erosion models

An experimental strategy, which is commonly used in water-ice impact studies, is utilized for the basic particle breakup experiments in this study. The well-established dynamic-indentation technique is used in a novel context to experimentally assess erosive airfoil defouling.
1.3 Research design

This work’s core content is subdivided into seven main chapters and the structure of the study is shown in Fig. 1.4. Firstly, Chapter 2 comprises a general introduction into the physical background of continuous and dispersed phase modelling as well as a brief introduction into axial compressor physics. Chapter 3 contains a detailed literature review on compressor fouling and cleaning, dry-ice injection system modelling, particle breakup modelling and defouling erosion modelling and it concludes with a summary of the most important findings from this survey to this work.

![Diagram of research design and structure](image-url)

**Figure 1.4.** Overview of the structure of this work with references to the corresponding chapters.
The study then splits into three main strands dealing with dry-ice injection system modelling in Chapter 4, with the development of a new particle breakup model for dry-ice in Chapter 5 and with the development of a new defouling erosion model in Chapter 6. In all these parts of the study theoretical, experimental and numerical approaches are considered. Both the new models are tested and compared to reality in a specially designed wind-tunnel experiment and this is described in Chapter 7. Finally, all the above findings are used to simulate actual engine defouling and this is described in Chapter 8. These simulations are partially compared to experiments carried out at the test-rig.
2 Physical background

A general introduction is given into the approach used in this work to assess relevant physical phenomena. After presentation of a general physical classification methodology in section 2.1, later Subsections 2.1.1 and 2.1.2 present general governing equations and use the classification methodology to simplify the general approach to final model assumptions valid to describe physics encountered in this work. Problem specific phenomena are then presented in the general context of dry-ice injection systems in section 2.1 and for axial aircraft compressor flows in section 2.3. All information given in this Chapter is, unless otherwise specified, taken from [24, 53, 93, 163, 165, 177].

2.1 General problem classification

Fluid flow phenomena considered in this work are assumed to be continuous. This assumption is justified if the Knudsen number, $Kn$, which is defined as quotient of a characteristic molecular length scale $\lambda^*$ of the fluid and a characteristic geometrical length scale $L^*$ of the problem investigated is lower than $10^{-2}$

$$Kn := \frac{\lambda^*}{L^*}.$$  \hspace{1cm} (2.1)

It is assumed that this statement is valid in all flow situations considered in this work.

By means of the Mach number

$$Ma := \frac{u}{a}$$  \hspace{1cm} (2.2)
which relates fluid bulk velocity $u$ to the sonic velocity $a$, it can be determined whether or not compressibility effects are negligible. The fluid’s sonic velocity can be expressed as a function of temperature $T$

$$a = \left[\kappa \cdot R_s \cdot T \right]^{\frac{1}{2}}$$

if it is assumed that the flow is isentropic and the fluid is an ideal gas. This permits usage of isentropic exponent $\kappa$ and specific gas constant $R_s = 287 \text{ J} / (\text{kg} \cdot \text{K})$. The ideal gas equation is used to relate density $\rho$ to pressure $p$ and temperature

$$\rho = \frac{p}{R_s \cdot T}.$$ 

A sample classification of flows by means of Mach number is shown in Tab. 2.1.

<table>
<thead>
<tr>
<th>Range</th>
<th>Example</th>
<th>Flow State</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Ma \leq 0.25$</td>
<td>blower</td>
<td>subsonic, incompressible</td>
</tr>
<tr>
<td>$0.25 &lt; Ma &lt; 1.00$</td>
<td>compressor</td>
<td>subsonic, compressible</td>
</tr>
<tr>
<td>$1.00 \leq Ma &lt; 5.00$</td>
<td>dry-ice nozzle</td>
<td>supersonic, compressible</td>
</tr>
<tr>
<td>$5.00 &lt; Ma$</td>
<td>rocket-engine</td>
<td>hypersonic, compressible</td>
</tr>
</tbody>
</table>

**Table 2.1.:** Typical flow classification by means of Mach number.

Using the above classification there are three Mach number regimes applicable to this work. These are subsonic incompressible, compressible and supersonic compressible.

The general flow state of a fluid flow can be classified by means of the Reynolds number

$$Re := \frac{\rho \cdot u \cdot L^*}{\eta}$$

and it represents the quotient of inertia contributions to viscous contributions to the momentum conservation and gives a measure for the degree of turbulence.
in a flow. The number incorporates fluid’s dynamic viscosity \( \eta \) and a characteristic length scale of the problem, for example the diameter of a pipe if investigating a piping flow. It must be noted that classification of a flow state using the Reynolds number is highly dependent on the geometry considered, which mainly influences the definition of the problem-specific characteristic length scale. Table 2.2 summarizes some typical Reynolds number ranges and gives corresponding examples.

<table>
<thead>
<tr>
<th>Range</th>
<th>Example</th>
<th>Turbulence State</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Re \ll 1 )</td>
<td>micro-channels</td>
<td>laminar creeping flow</td>
</tr>
<tr>
<td>( 1 &lt; Re &lt; 2.3 \cdot 10^3 )</td>
<td>pipe flow - low velocity water supply</td>
<td>laminar flow</td>
</tr>
<tr>
<td>( 2.3 \cdot 10^3 \leq Re \leq 1.0 \cdot 10^4 )</td>
<td>pipe flow - transient process petrochemical plant</td>
<td>transition zone</td>
</tr>
<tr>
<td>( 1.0 \cdot 10^4 &lt; Re )</td>
<td>pipe flow - acceleration dry-ice nozzle</td>
<td>turbulent flow</td>
</tr>
<tr>
<td>( Re \rightarrow \infty )</td>
<td>aircraft at high altitude</td>
<td>inviscid flow (turbulent)</td>
</tr>
</tbody>
</table>

**Table 2.2.:** Typical flow classification by means of Reynolds number.

The nozzle and free jet flows considered in this work are turbulent. Many researchers experimentally investigated the relationship between a frictional loss coefficient \( \zeta \) and the Reynolds number. This loss coefficient is used for determination of roughness induced pressure losses in pipe flows (here the pipe is characterized by its length \( L \) and diameter \( d \)):

\[
\delta p_v = \zeta \cdot \frac{L}{d} \cdot \frac{\rho}{2} \cdot u^2.
\] (2.6)

Various characteristic dependencies are listed in [179] and those for flows through rough pipes are shown in Fig. 2.1 and discussed below.
Figure 2.1.: Frictional loss coefficient as function of Reynolds number for pipes with various roughness, graph from [100].

Actual roughness values $k_r$ are related to pipe diameters in the above diagram and the resulting equivalent roughness values

$$\varepsilon_r = \frac{k_r}{d} \quad (2.7)$$

are curve parameters. The following functional dependencies were found:

- $Re < 2.3 \cdot 10^3$ - laminar flow - $\zeta = f \left( Re \right)$
- $2.3 \cdot 10^3 \leq Re \leq 1.0 \cdot 10^4$ - transition zone - $\zeta = f \left( Re, k_r \right)$
- $1.0 \cdot 10^4 < Re$ and $k_{crit} < k_r$ - fully turbulent flow - $\zeta = f \left( k_r \right)$

and it is shown that the nature of frictional losses is highly dependent on the general flow state, which is characterized by Reynolds number as discussed above.

Heat transfer in flows can be classified in general utilizing the Rayleigh number

$$Ra := Gr \cdot Pr \quad (2.8)$$
which is a product of the Grashof number

\[ Gr := g \cdot \frac{L^3}{\eta} \cdot \rho \cdot \beta \cdot (\delta T^*) \]  \hspace{1cm} (2.9)

accounting for gravity \( g \), thermal expansion coefficient \( \beta \) and a characteristic driving temperature difference \( \delta T^* \) and the Prandtl number

\[ Pr := \frac{\eta}{\rho \cdot \alpha} \]  \hspace{1cm} (2.10)

which relates viscous contributors to conductive contributors of the heat transfer regime. The latter are represented by the temperature conductivity \( \alpha \).

By means of the Rayleigh number it can be determined whether or not natural convection is negligible in a fluid flow. For the flow phenomena considered here it is assumed that forced convection is the main influence on heat transfer, hence natural convection remains neglected.

For the dispersed phase (i.e. particles) the Stokes number

\[ St := \frac{\tau_p}{\tau_F} \]  \hspace{1cm} (2.11)

determines the particle’s kinematic dependence on the surrounding fluid. It relates a characteristic particulate time scale \( \tau_p \) to a characteristic fluid flow time scale \( \tau_F \). The following Tab. 2.3 provides an overview of typical Stokes number ranges.

<table>
<thead>
<tr>
<th>Range</th>
<th>Example</th>
<th>Particle Behaviour</th>
</tr>
</thead>
<tbody>
<tr>
<td>( St \ll 1 )</td>
<td>PIV seeding particles</td>
<td>ideally following the flow</td>
</tr>
<tr>
<td>( St \approx 1 )</td>
<td>industrial granules</td>
<td>either possibility</td>
</tr>
<tr>
<td>( 1 \ll St )</td>
<td>hail particles</td>
<td>tracks independent from flow</td>
</tr>
</tbody>
</table>

Table 2.3: Examples of particle laden flows and Stokes number ranges.
Stokes numbers from all the above regimes are encountered in the particle laden flows considered in this work. The classification procedures presented here are used below to simplify the general governing equations to a basic set of equations applicable for physical descriptions in this work.

2.1.1 Fluid phase modelling

Assuming any physical quantity $\Phi$ to be defined as:

$$\Phi = \int \int \int_{V(t)} \phi dV$$  \hspace{1cm} (2.12)

if considering a continuum belonging to the range of Knudsen numbers $Kn < 10^{-2}$ (see above Eqn. (2.1)) and regarding this in a global manner leads to the general governing equation for a substantial volume $V(t)$ which is surrounded by its boundary $\partial V(t)$ and which contains the above defined quantity $\Phi$

$$\frac{d\Phi}{dt} = -O + Z + P.$$  \hspace{1cm} (2.13)

Transient changes of the quantity $\Phi$ are balanced as a function of the flowing, feeding and productive contributions $O$, $Z$ and $P$. This physical relation can be written explicitly as:

$$\frac{d\Phi}{dt} = \frac{d}{dt} \int \int \int_{V(t)} \phi dV = -\int \int \left( \mathbf{a} \cdot \mathbf{n} \right) dS + \int \int \int_{V(t)} z^{(\phi)} dV + \int \int \int_{V(t)} p^{(\phi)} dV$$ \hspace{1cm} (2.14)

and it is defined as the Lagrange equation (i.e. volume-specific). It contains, as mentioned above, transient changes of the quantity $\phi$

$$\frac{d\Phi}{dt} = \frac{d}{dt} \int \int \int_{V(t)} \phi dV$$ \hspace{1cm} (2.15)
which are dependent on the flow of $\phi$ over the volumes boundary $\partial V(t)$

$$O = \int \int_{\partial V(t)} (o^{\{\phi\}} \cdot n) \, dS,$$  \hspace{1cm} (2.16)

on external sources of $\phi$

$$Z = \int \int \int_{V(t)} z^{\{\phi\}} \, dV,$$ \hspace{1cm} (2.17)

and from production sources of $\phi$ inside the volume

$$P = \int \int \int_{V(t)} p^{\{\phi\}} \, dV.$$ \hspace{1cm} (2.18)

Typical examples for contributors to this general physical balancing approach are listed in Tab. 2.4.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Explanation</th>
<th>Physical Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi$</td>
<td>physical quantity</td>
<td>mass, momentum, energy</td>
</tr>
<tr>
<td>$O$</td>
<td>flow of $\phi$ over $\partial V(t)$</td>
<td>convective transport of $\Phi$</td>
</tr>
<tr>
<td>$Z$</td>
<td>external source of $\phi$</td>
<td>gravity, radiation</td>
</tr>
<tr>
<td>$P$</td>
<td>internal production of $\phi$</td>
<td>heat-source, mass-source (i.e. by chemical reaction)</td>
</tr>
</tbody>
</table>

**Table 2.4.:** Contributors to general Lagrangian balancing Eqn. (2.14).

Application of Reynolds transportation theorem and Gaussian integration rules as well as change from the global Lagrange formulation to the local Eulerian formulation (i.e. space-specific) leads to the following rewritten form of Eqn. (2.14):

$$\int \int \int_{V(t)} \left[ \frac{d\phi}{dt} + \nabla \cdot (\phi \cdot u) + \nabla \cdot o^{\{\phi\}} - z^{\{\phi\}} - p^{\{\phi\}} \right] \, dV = 0$$  \hspace{1cm} (2.19)
from which the general local balancing equation can be derived:

$$\frac{d\phi}{dt} + \nabla \cdot (\phi \cdot u) + \nabla \cdot o\{\phi\} - z\{\phi\} - p\{\phi\} = 0. \quad (2.20)$$

Substitution of appropriate physical quantities in this formulation leads to a set of governing equations, which is used within this work to describe all fluid flows. Table 2.5 summarizes these quantities.

<table>
<thead>
<tr>
<th>Equation</th>
<th>Variable $\phi$</th>
<th>$o{\phi}$</th>
<th>$z{\phi}$</th>
<th>$p{\phi}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MASS</td>
<td>$\rho$</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>MOMENTUM</td>
<td>$\rho \cdot u$</td>
<td>$T$</td>
<td>$\rho \cdot g$</td>
<td>0</td>
</tr>
<tr>
<td>ENERGY</td>
<td>$\frac{1}{2} \rho \cdot (u \cdot u) + \rho \cdot e$</td>
<td>$uT - q$</td>
<td>$\rho \cdot (g \cdot u)$</td>
<td>$\rho \cdot \dot{s}$</td>
</tr>
<tr>
<td>ANGULAR MOMENTUM</td>
<td>$x \times (\rho \cdot u)$</td>
<td>$x \times T$</td>
<td>$x \times (\rho \cdot g)$</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 2.5.** Contributors to general Eulerian balancing Eqn. (2.20).

Application of these quantities leads to the describing set of Cauchy differential equations, i.e. the mass-balance

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \cdot u) = 0, \quad (2.21)$$

the momentum-balance

$$\frac{d (\rho \cdot u)}{dt} + \nabla \cdot ([\rho \cdot u] \times u) = \nabla \cdot T + \rho \cdot g, \quad (2.22)$$

and the energy-balance

$$\frac{d \rho \left(\frac{1}{2} [u \cdot u] + e\right)}{dt} + \nabla \cdot \left(\rho \left(\frac{1}{2} [u \cdot u] + e\right) \cdot u\right) = \ldots$$

$$\ldots \text{tr} \left(T \cdot \frac{1}{2} \left[\nabla u + (\nabla u)^T\right]\right) - \nabla \cdot q + \rho \cdot (g \cdot u) + \rho \cdot \dot{s}. \quad (2.23)$$
Angular momentum remains neglected here because it is used only in the final application case simulations and it can be derived from the momentum-balance Eqn. (2.22).

To complete this set of differential equations appropriate material models and closure assumptions must be applied. The first variable from the above set of equations to be modelled is density. For the scope of this work, all fluids modelled are gases and the ideal gas formulation, Eqn. (2.4), is used. It assumes that a fluid’s density is a function of pressure and temperature.

Assuming all fluids modelled in this work can be described by Newton’s stress tensor; this material stress tensor is defined as:

\[
T = -pI + \mu^* \nabla \cdot uI + \eta \left( \nabla u + (\nabla u)^T \right) - \frac{2}{3} \left( \nabla \cdot u \right) \cdot I.
\]  

Here the first contribution to the right-hand side specifies pressure contributions, the second term represents compressibility effects and the third contribution to the right-hand side represents fluid dynamic viscosity effects. The incorporated material properties are volumetric viscosity \( \mu^* \) and dynamic viscosity \( \eta \) and these are treated as constants within this work.

Acceleration due to gravity \( \mathbf{g} \) is also treated as constant and is:

\[
\mathbf{g} = (0, 0, -9.81)^T
\]

assuming a global Cartesian coordinate system with its third component being the earth’s normal vector.

Internal energy \( e \) is modelled integrating the general definition

\[
de = c_v(T) \, dT
\]

with respect to temperature assuming the specific heat capacity \( c \) to be constant in the scope of this work and assuming the integration constant to be zero:

\[
e = c_v \cdot T.
\]
Fourier’s law is used to describe the heat conductivity inside the fluid

\[ \mathbf{q} = -\lambda \cdot \nabla T. \]  

(2.28)

This equation incorporates the material’s thermal conductivity \( \lambda \) which is also treated as a constant in this work.

The last two contributions to the right-hand side of the energy-balance, Eqn. (2.23), remain neglected in all cases considered here. These are potential energy contributions, which are assumed to be small compared to all other contributions and energy sources or sinks, which are not applied since no chemical reactions are modelled. In the case of modelling sublimation of CO\(_2\) dry-ice particles, the above set of differential equations is applied to gaseous CO\(_2\) and a mixture model is used.

**Treatment of turbulence**

If the flow is turbulent (using Reynolds number classification), which is the case for all flow situations considered in this work, instantaneous physical quantities (here in an overall stationary case) can be written as a sum of mean values \( \bar{\phi} \) and fluctuations \( \tilde{\phi} \):

\[ \phi(x, t) = \bar{\phi}(x) + \tilde{\phi}(x, t) \]  

(2.29)

where mean values can be derived from a time averaging procedure

\[ \bar{\phi}(x) = \frac{1}{T} \int_{0}^{T} \phi(x, t) \, dt \]  

(2.30)

taking into account an averaging time-scale (here: \( T \)) which is much higher than the characteristic time-scale of turbulent fluctuations, i.e. \( T \gg t^* \). Using this procedure for all the balancing equations given above averages all but
one physical quantity. The averaging of convective terms of the momentum-balances, Eqn. (2.22), form an additional contributor, which results from the cross-product of the velocity field:

$$\nabla \cdot (\rho \cdot \mathbf{u} \times \mathbf{u}) = \nabla \cdot (\rho \cdot \bar{\mathbf{u}} \times \bar{\mathbf{u}}) + \nabla \cdot (\bar{\rho} \cdot \bar{\mathbf{u}} \times \bar{\mathbf{u}}) .$$

(2.31)

This additional contribution is defined to be the Reynolds stress tensor:

$$\mathbf{T}_R = -\nabla \cdot (\bar{\rho} \cdot \bar{\mathbf{u}} \times \bar{\mathbf{u}}) .$$

(2.32)

This fluctuation relation resulting from the above averaging procedure is of convective nature and it is physically comparable to the stress-strain relations in a laminar flow. There is a range of approaches to model or directly simulate these additional turbulent stresses, such as Reynolds Averaged Navier Stokes Equations Modelling (RANS), Large Eddy Simulation (LES), Detached Eddy Simulation (DES) etc.

Here, RANS modelling applying the gradient assumption is used, which is based on the Boussinesque eddy viscosity assumption. It states that the additional Reynolds stresses can be obtained from velocity gradients, which are averaged with the above procedure, Eqn. (2.30). The structure of the Reynolds' stress tensor is therefore comparable to the Newton's stress tensor, Eqn. (2.24), and can be written as

$$\mathbf{T}_R \approx \eta_{turb} \cdot \left[ \nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^T \right] - \frac{2}{3} \cdot \bar{\rho} \cdot \bar{k} + \eta_{turb} \cdot \nabla \cdot \bar{\mathbf{u}} \cdot \mathbf{I} .$$

(2.33)

and it contains the turbulent kinetic energy:

$$k = \frac{1}{2} (\bar{\mathbf{u}} \cdot \bar{\mathbf{u}}) .$$

(2.34)

Furthermore, turbulent viscosity $\eta_{turb}$ is contained in Eqn. (2.33) and it is not a material property but a flow quantity. It must be modelled to achieve closure and modelling approaches are discussed below.
Finally the Newton’s stress tensor $T$, Eqn. (2.24), which is used in the momentum and energy-balance equations, is modified applying the Reynolds stresses:

$$T' = T + T_R.$$ (2.35)

There are several models available for the formulation of turbulent viscosity and most of them are empirical or semi-empirical. Two such models are considered in this work: the Ansys CFX implementation of the classical $k-\epsilon$ model, which was presented originally by LAUNDER and SPALDING in 1974 [107] and the SST model presented by MENTER et al. in 1993 [121].

Using the $k-\epsilon$ approach, turbulence eddy dissipation must be calculated as second additional field variable, which is defined as

$$\epsilon := \frac{\eta}{\rho} \cdot (\nabla \bar{u} \cdot (\nabla \bar{u})^T)$$ (2.36)

and with this, turbulent viscosity can be calculated using to the Kolmogorov-Prandtl relation

$$\eta_{turb} = C_\eta \cdot \bar{\rho} \cdot \frac{k^2}{\epsilon}$$ (2.37)

and utilizing one of the model’s constants $C_\eta$. It must be noted that the velocity divergence term on the right-hand side of the Reynolds stress tensor, Eqn. (2.33), is neglected in the model. This assumption is in general correct for incompressible flows only.

Transport equations of a similar structure as reported above (see general Eulerian Eqn. (2.20)) must be solved to obtain $k$

$$\frac{d (\rho \cdot k)}{dt} + \nabla \cdot (\rho \cdot \dot{k} \cdot \dot{u}) = \nabla \cdot \left[ \left( \eta + \frac{\eta_{turb}}{\sigma_k} \right) \cdot \nabla k \right] + p^{[k]} + p^{[kk]} - \rho \cdot \epsilon$$ (2.38)
and \(\epsilon\)

\[
d \left( \rho \cdot \epsilon \right) \frac{d}{dt} + \nabla \cdot \left( \rho \cdot \epsilon \cdot \mathbf{u} \right) = \nabla \cdot \left[ \left( \eta + \frac{\eta_{turb}}{\sigma_\epsilon} \right) \cdot \nabla \epsilon \right] + \frac{\epsilon}{k} \cdot C_{\epsilon_1} \cdot \left[ p^{[k]} + p^{[\epsilon b]} \right] - \frac{\epsilon}{k} \cdot C_{\epsilon_2} \cdot \rho \cdot \epsilon
\]  

(2.39)

from a numerical solution process. The production terms on the right-hand side of both above equations represent:

- \(p^{[k]}\) = turbulence production induced by viscous forces
- \(p^{[kb]}\) and \(p^{[\epsilon b]}\) = influence of buoyant forces

and they contain a number of additional modelling constants. Formally, the model must be calibrated by means of basic experiments depending on the application. However, the default model constants reported in [107] mostly work well in various situations and these are also used in this work and are listed in Tab. 2.6.

<table>
<thead>
<tr>
<th>Constant</th>
<th>(C_\eta)</th>
<th>(\sigma_k)</th>
<th>(\sigma_\epsilon)</th>
<th>(C_{\epsilon_1})</th>
<th>(C_{\epsilon_2})</th>
<th>(C_{p_k})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.09</td>
<td>1.00</td>
<td>1.30</td>
<td>1.44</td>
<td>1.92</td>
<td>3.00</td>
</tr>
</tbody>
</table>

**Table 2.6.:** Default model constants of the \(k - \epsilon\) turbulence model.

One of the main disadvantages of the above \(k - \epsilon\) turbulence model is the near wall treatment for low Reynolds number flows [120, 121, 122, 206]. Therefore WILCOX [206] presented the \(k - \omega\) turbulence model, which accounts for eddy frequency \(\omega\) instead of eddy dissipation

\[
\omega = \frac{1}{C_{\omega 0} \cdot \frac{\epsilon}{k}}
\]  

(2.40)

and with this, turbulent viscosity is calculated in a different way

\[
\eta_{turb} = \bar{\rho} \cdot \frac{k}{\omega}.
\]  

(2.41)
The $k - \omega$ model uses the same Reynolds stress assumption as the above $k - \epsilon$ model, Eqn.(2.33) and (2.35), and the equations to be solved for the model variables are those for $k$:

$$
\frac{d (\rho \cdot k)}{dt} + \nabla \cdot ([\rho \cdot k] \cdot \mathbf{u}) = \nabla \cdot \left[ \left( \eta + \frac{\eta_{turb}}{\sigma_k} \right) \cdot \nabla k \right] + \mathbf{p}^{[k]} + \mathbf{p}^{[kb]} - C_{\omega 0} \cdot \rho \cdot k \cdot \omega \quad (2.42)
$$

and $\omega$:

$$
\frac{d (\rho \cdot \omega)}{dt} + \nabla \cdot ([\rho \cdot \omega] \cdot \mathbf{u}) = \nabla \cdot \left[ \left( \eta + \frac{\eta_{turb}}{\sigma_\omega} \right) \cdot \nabla \omega \right] + \frac{\omega}{k} \cdot C_{\omega 1} \mathbf{p}^{[k]} + \mathbf{p}^{[\omega b]} - C_{\omega 2} \cdot \rho \cdot \omega^2 \quad (2.43)
$$

which are obtained from a numerical solution process. The source terms on the right-hand side of both above equations are comparable to what is reported for the $k - \epsilon$ source terms discussed above. The default model constants are given in Tab. 2.7.

<table>
<thead>
<tr>
<th>Constant</th>
<th>$\sigma_k$</th>
<th>$\sigma_\omega$</th>
<th>$C_{\omega 0}$</th>
<th>$C_{\omega 1}$</th>
<th>$C_{\omega 2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>2.00</td>
<td>2.00</td>
<td>0.09</td>
<td>5/9</td>
<td>0.075</td>
</tr>
</tbody>
</table>

**Table 2.7:** Default model constants of the $k - \omega$ turbulence model.

MENTER [121] reported a particular sensitivity of the WILCOX model to free stream conditions. Therefore, he suggested to blend both above presented turbulence models depending on the distance from walls to benefit from free-flow advantages of the $k - \epsilon$ model and near wall advantages of the $k - \omega$ model:

$$
\phi = F_1 \cdot \phi^{[k-\epsilon]} + (1 - F_1) \cdot \phi^{[k-\omega]}.
$$

(2.44)
This blending procedure is in principle shown above using the replacement variable $\phi$ which represents in this case $k$, $\epsilon$ and $\omega$. The blending function can be found in [120] and its functional relation is:

$$F_1 = \tanh \left[ \log \left( k, \nabla k, \nabla \omega, \rho, \eta, C_{\omega 0}, \sigma, y \right) \right]$$

(2.45)

where $y$ denotes the minimum wall distance of a current numerical node.

A further important modification by MENTER [122] to the above blending procedure resulted in the $SST$ model. It accounts for shear stress transport and eliminates the main disadvantage of the above hybrid model, Eqn. (2.45), which was reported to be prone to false predictions of flow separation from smooth surfaces under influence of adverse pressure gradients. Due to MENTER, the above hybrid model overpredicts eddy-viscosity. Therefore, the eddy-viscosity formulation was modified applying a source term limiter

$$\eta_{turb} = \bar{\rho} \cdot \frac{C_{\omega 1} \cdot k}{\max \left( C_{\omega 1} \cdot \omega, S \cdot F_2 \right)}$$

(2.46)

and clipping it to the wall boundary layer by means of an appropriate blend function

$$F_2 = \tanh \left[ \log \left( k, \omega, \rho, \eta, C_{\omega 0}, y \right) \right] .$$

(2.47)

Treatment of boundary layers

In the vicinity of solid walls the no-slip condition applies to Newtonian fluids, as considered in this work. Therefore a boundary layer develops, in which the flow velocity gradually increases from wall-velocity to free-flow velocity. These relations are shown schematically in Fig. 2.2 for a flow parallel to a horizontal flat plate according to SCHLICHTING and GERSTEN [167].
In this boundary layer an analytical solution to the above balancing equations for Newtonian fluids and subsonic flow was derived by PRANDTL in 1904 [167]. It is based on the general assumption that, even if an inviscid flow can be considered in the far field (i.e. inertial forces are much bigger than viscous forces, \( Re_\infty \rightarrow \infty \)), this situation changes significantly near the wall, where it is assumed that inertial forces

\[
\rho \cdot u \cdot \frac{\partial u}{\partial x} \sim \rho \frac{u_\infty^2}{x} \quad (2.48)
\]

and viscous forces

\[
\frac{\partial \tau}{\partial y} \sim \frac{u_\infty}{\delta^2} \quad (2.49)
\]

are of the same order of magnitude

\[
\rho \frac{u_\infty^2}{x} \sim \frac{u_\infty}{\delta^2} \quad (2.50)
\]

This modifies the order of the descriptive Reynolds number from free flow to near wall regimes as follows:

\[
\Theta (Re) = \infty \rightarrow \Theta (Re) = 1 \quad (2.51)
\]
and it is obvious that a possible inviscid flow assumption for the far field cannot be valid near solid walls.

Rearrangement of the above relation, Eqn. (2.50), leads to the following estimating formulation for laminar boundary layer thickness

\[ \delta_{99} \sim \left[ \frac{\eta}{\rho \cdot u_{\infty}} \right] \frac{1}{2}. \] (2.52)

Further usage of this in a relation to a characteristic length of the area (here a flat plate) and derivation of the proportionality factor (details can be found in [167]) leads to

\[ \frac{\delta_{99}(x)}{L^*} \approx \frac{5}{\sqrt{Re_{L^*}}} \cdot \left[ \frac{x}{L^*} \right] \frac{1}{2}. \] (2.53)

Following Newton’s law, wall shear stresses can be determined using a linear velocity gradient estimate

\[ \tau_w(x) = \eta \cdot \left( \frac{\partial \tilde{u}}{\partial y} \right)_w \approx \eta \cdot \left( \frac{u_{\infty}}{\delta_{99}} \right), \] (2.54)

and application of Eqn. (2.52) in the above formulation leads to an approximate relation of the wall shear stresses:

\[ \tau_w(x) \sim \left[ \frac{\eta \cdot \rho \cdot u_{\infty}^3}{x} \right] \frac{1}{2}. \] (2.55)

A critical Reynolds number can be calculated to assess the change from laminar to turbulent boundary layer, which in case of a flat plate is a function of plate length and far-field flow pattern, combining the wall shear stress formulation and the Reynolds’ stress tensor introduced above (Eqn. (2.32)):

\[ \tau_w(x) = \eta \cdot \left( \frac{\partial \tilde{u}}{\partial y} \right)_w - \rho \overline{\tilde{u} \tilde{v}}. \] (2.56)
Rearrangement of this equation leads to the formulation of a shear stress velocity

\[ u_\tau = \left[ \frac{\tau_w}{\rho} \right]^{\frac{1}{2}} = \left[ \frac{\eta}{\rho} \left( \frac{\partial \bar{u}}{\partial y} \right)_w - \bar{u} \cdot \bar{v} \right]^{\frac{1}{2}} \quad (2.57) \]

which is a measure for turbulent fluctuations.

The development of velocity components \( u \) tangential to the wall can be described by means of the logarithmic wall function, which relates the dimensionless tangential velocity component

\[ u_+ = \frac{\bar{u}}{u_\tau} \quad (2.58) \]

to the dimensionless wall distance (which can be interpreted also as a Reynolds number)

\[ y_+ = \frac{u_\tau \cdot y}{\nu}. \quad (2.59) \]

Following LAUNDER and SPALDING [107] and their basic implementation of this relation into their turbulence model, this logarithmic wall law can be modelled

\[
    u_+ = \begin{cases} 
    y_+ & 1 \leq y_+ \leq 10 \\
    \frac{1}{\kappa} \cdot \ln (y_+) + B - \Delta B & 10 < y_+ \leq 1000 \\
    \left( \frac{u_\infty}{-\bar{u}} \right)^2 & 1000 < y_+ \end{cases} \quad (2.60)
\]

and it is used in this work with the Karman constant \( \kappa = 0.41 \) and the integration constant \( B = 5.2 \) in the scalable wall treatment implementation of Ansys CFX. This implementation neglects the viscous sub-layer (i.e. the first region \( 1 \leq y_+ \leq 10 \), for details see [9]).
Figure 2.3 illustrates the above regimes of the logarithmic wall law. It makes it possible to account for boundary layers in simulations in an approximate manner without the necessity to resolve the fine scales near the wall.

The additional shift factor $\Delta B_r$ in Eqn. (2.60) can be applied for rough walls and it can be expressed as a function of equivalent sand-grain roughness

$$\Delta B_r = \frac{1}{\kappa} \cdot \ln \left( 1 + 0.3 \cdot h_{+}^{[s]} \right)$$  \hspace{1cm} (2.61)

with the dimensionless sand-grain roughness height

$$h_{+}^{[s]} = \frac{u_{*} \cdot k_r}{\nu}$$  \hspace{1cm} (2.62)

which can be calculated by means of an actual representative roughness value $k_r$ following for example [167]. A possible narrowing effect from the roughness layer can be also considered assuming the wall’s height to be increased by half of the roughness height

$$y = \max \left( y, \frac{k_r}{2} \right).$$  \hspace{1cm} (2.63)
2.1.2 Solid phase modelling

All dispersed solid phase particles considered in this work are treated as single particles. Therefore a modified formulation of the classical BASSET [20], BOUSSINESQ [22], OSEEN [141] equation (BBO equation) presented by TCHEN [191] is used to model corresponding particle tracks. While the original BBO equation is valid only for spherical particles settling in a still fluid driven by gravity effects, Tchen’s modification makes it applicable to unsteady and non-uniform flows [85]:

\[ m_p \cdot \frac{\partial^2 x_p}{\partial t^2} = \sum_{i=1}^{n} F_i. \]  (2.64)

With this equation, which represents Newton’s first law, particle tracks \( x_p \) can be calculated in a Lagrangian formulation as a function of the sum of external forces \( F_i \) acting on this particle. Fluid properties are treated as if no particle were present and all forces act at the mass centre of the particle. Particles are assumed to be of negligible volume and are therefore treated as ideal and non-rotating spherical point masses of mass \( m_p \).

An overview of possible forces acting on such a single particle is given in Tab. 2.8, which also contains a classification of these forces into volumetric, flow-induced and particulate close-up forces following [53].

The particle velocity vector is

\[ v_p = \frac{dx_p}{dt} \]  (2.65)

and the most important force on the right-hand side of Eqn. (2.64) which must be considered in this work is the drag force:

\[ F_{\text{drag}} = \frac{1}{2} \cdot \frac{\pi}{4} \cdot d_p^2 \cdot \rho_f \cdot c_D \cdot |u - v_p| \cdot (u - v_p). \]  (2.66)
Table 2.8.: A number of typical forces acting on dispersed particles that can be considered in Eqn. (2.64).

It is composed differently from the original formulation of the Stokes drag force proposed by TCHEN [191] and it applies the cross-sectional area of the particle (here calculated from particles diameter \( d_p \)) and the drag coefficient \( c_D \). The latter is either a function of particle Reynolds number in subsonic flows

\[
Re_p = \frac{\left| \mathbf{u} - \mathbf{v}_p \right| \cdot d_p}{v}.
\]  

(2.67)

or a function of particle Reynolds and free-flow Mach numbers in transonic and supersonic flows (discussed in detail in section 2.2). Furthermore, it can be influenced by additional factors such as particle shape.

Various regimes must be considered for ideal spherical particles in subsonic flows and these are shown in Fig. 2.4 depending on the particle Reynolds number.

These regimes can be classified as follows:

- Stokes regime - \( Re_p < 1 \)
- transitional regime - \( 0.5 < Re_p < 1000 \)
Figure 2.4.: Drag coefficient as function particle Reynolds number for spherical particle in subsonic regime, diagram from [129].

- Newton regime \(-1000 < Re_p < 2.5 \cdot 10^5\)
- critical regime \(-2.5 \cdot 10^5 < Re_p < 4.0 \cdot 10^5\)
- supercritical regime \(-4.0 \cdot 10^5 < Re_p\)

and there are numerous correlations available in the literature for each of these regimes. In this work, the drag coefficient is calculated by the modified Schiller-Naumann formulation (comparable to what is reported in [106]):

\[
c_D = \max \left[ \frac{24}{Re_p} \cdot \left(1 + 0.15 \cdot Re_p^{0.687} \right), 0.44 \right]
\]

(2.68)

and this is valid for subsonic flows up to the critical regime. Possibly necessary modifications to the drag coefficient in transonic and supersonic dry-ice blasting flows are presented and discussed in section 4.5.

Moreover, buoyant (or gravitational) force, which also includes static pressure contributions of the surrounding fluid

\[
F_g = (m_p - m_f) \cdot g
\]

(2.69)
and pressure-gradient force

\[
F_{dp} = -\nabla p \cdot \frac{m_p}{\rho_p}.
\]  

are considered.

Further possible force contributions to Eqn. (2.64) such as those listed in Tab. 2.8 remain neglected. These include for example the Basset force, accounting for transient boundary layer effects at particle surfaces, or the added mass force, accounting for displaced and accelerated proportions of the surrounding fluid.

Neglecting these forces is usually valid for situations where particle density is much higher than fluid density [53], which is the case in all situations discussed in this work. Turbulence dispersion force is also neglected, because only single particles (such as in the validation case presented in section 4.2) or particle classes (such as in the parameter studies presented in section 4.4 and in the application case presented in Chapter 8) with turbulence-specific Stokes numbers much greater than unity are considered [65, 106].

In case of the turbulent dispersion force, turbulent structure turnover times must be considered in the denominator of the Stokes number, Eqn. (2.11). Details about this can be found for example in the publications by ELGHOBASHI [50, 51].

Applied phase coupling

The Lagrangian particle tracking approach presented above is formally valid for the Stokes regime if the following restrictive relations are found for a particular physical situation according to [115].
The characteristic size \( r_p \) of the particles must be much smaller than a critical characteristic length \( L^* \) of the flow channel

\[
\frac{r_p}{L^*} \ll 1, \tag{2.71}
\]

and inertial forces acting on the particle must be much less important than viscous forces

\[
\frac{r_p \cdot (|u - v_p|)}{\nu} \ll 1. \tag{2.72}
\]

However, the Lagrangian particle tracking approach is much more widely used and there is a number of force models which deliver good predictions for the other regimes discussed above. Therefore the approach is used in this work even if the restrictions (i.e. Eqn. (2.71) and (2.72)) indicate that a much more complicated or numerically expensive particle tracking methodology, such as an Euler-Euler approach described in [53, 68, 85, 106] or a modified Boltzmann approach described in [68, 85], must be used.

With the Lagrangian equation, there are two ways to couple solid and fluid phases. The simplest is the one way coupling strategy (1-wc), where particle tracks are calculated by integrating particle ODEs of motion, Eqn. (2.64), driven by an already known (or numerically calculated) flow-field. There are no modifications made to the governing equations of the fluid phase, which is estimated a-priori.

If particles can significantly influence the fluid phase, there are additional contributors to be considered in these equations, and this method is called two way coupling (2-wc). In the formulation chosen for this work (i.e. the Ansys CFX implementation), there is a modification considered in the momentum equations if 2-wc is used:

\[
\frac{d (\rho \cdot u)}{dt} + \nabla \cdot (\rho \cdot [u] \times \mathbf{u}) = \nabla \cdot \mathbf{T} + \rho \cdot \mathbf{g} - p^{p \leftrightarrow f}. \tag{2.73}
\]
An additional source term \( \mathbf{p}^{[P \rightarrow F]} \) is applied to the equation’s right-hand side and it accounts for particle influence upon the fluid phase.

Possible interactions of particles with turbulent structures are neglected in this work. Particle wall interaction is discussed for non-disintegrating and disintegrating particles in detail in section 3.3, because the introduction of a new particle breakup model for Lagrangian particle tracking of \( \text{CO}_2 \) dry-ice is one of the key novel developments presented in this work.

### 2.2 Injection system physics

Injection systems used in dry-ice blasting applications are often operated with convergent-divergent blasting nozzles. In these nozzles, dry-ice particles are accelerated in transonic flow conditions (see Tab. 2.1) for cleaning purposes. Figure 2.5 shows such a situation and highlights the main features of this type of flow, which must be considered in any adequate simulation approach.

These main features are:

- compressible, turbulent air flow
- supersonic outlet flow leading to over- or underexpanding jets

![Figure 2.5: Schematic of dry-ice laden flow through typical dry-ice blasting nozzle.](image-url)
• development of shocks and expansion and compression waves
• non-adiabatic thermodynamic behaviour
• particle-flow interaction

If pure air flow is considered, compressible effects inside the nozzle can be captured using an isentropic assumption which relates the fluids’ sonic velocity to pressure changes with respect to density:

\[ a^2 = \left( \frac{\partial p}{\partial \rho} \right)_{s=\text{const.}} \]  \hspace{1cm} (2.74)

A function of Mach number and local cross-sectional area \( A(x) \) of the nozzle can be derived:

\[ \frac{1}{u} \frac{du}{dx} \cdot (1 - Ma^2) = -\frac{1}{A(x)} \frac{dA}{dx} \]  \hspace{1cm} (2.75)

using the above expression for fluid sonic velocity in a one-dimensional differential mass-balance from Eqn. (2.21). This function makes it is possible to capture mean flow quantities inside convergent-divergent nozzles. Its full derivation can be found for example in [177].

Three typical flow states of convergent-divergent nozzles are shown in Fig. 2.6 and can be described as follows: the uppermost scheme shows flow acceleration in the subsonic convergent part of the nozzle, Mach number 1 at the throat position and further flow acceleration in the supersonic divergent part. If the nozzle pressure ratio is not sufficient the whole nozzle operates in subsonic flow conditions and this situation is shown in the middle scheme in Fig. 2.6. The flow is accelerated in the subsonic convergent part and decelerated in the subsonic divergent part of the nozzle. If the flow state at the inlet of the nozzle is already supersonic, the flow is decelerated in the convergent part and accelerated again in the divergent part of the nozzle and this situation is shown schematically at the bottom.
Figure 2.6.: Typical flow states of compressible flows through convergent-divergent nozzles.

Figure 2.7.: Possible compressible flow states inside a convergent-divergent nozzle depending on pressure setting, figure from [177] with modified nomenclature.
From the above it is clear that the flow velocity inside a convergent-divergent nozzle depends on Mach number regimes before and after the nozzle’s throat. These Mach numbers can be controlled by means of nozzle pressure. Figure 2.7 shows possible flow states inside a convergent-divergent nozzle depending on the relation of exit pressure $p_e$ to ambient pressure $p_a$.

Four pressure related flow states of such nozzles can be diversified:

- $p^* < p_a$ - subsonic nozzle behaviour - subsonic outlet - curve (1)
- $p^* \approx p_a$ - no supersonic flow establishment - subsonic outlet - curve (2)
- $p_x \approx p_a$ - expansion inside divergent part - subsonic outlet - curve (3)
- $p_e = p_a$ - ideal expanding nozzle - supersonic outlet - curve (4)

Thermodynamic properties of such flows can be balanced by means of isentropic relations between pressure and density assuming a calorically-perfect gas

\[ p = C \cdot \rho^\kappa \]  \hspace{1cm} (2.76)

and relating these quantities with a constant $C$ and the isentropic exponent $\kappa$. Fluid sonic velocity can be calculated with this expression in conjunction with an energy balance:

\[ a^2 = \kappa \cdot \frac{p}{\rho} \]  \hspace{1cm} (2.77)

With the above isentropic expressions, static flow variables (i.e. represented by $\phi$ being $\phi = a$, $T$, $\rho$, $p$ in a fluid at rest, index: $t = $ total) are related to those at any flow state as a function of Mach number (explicit expressions can be found for example in [177])

\[ \frac{\phi_t}{\phi} = f \left( \frac{\kappa - 1}{2} \cdot Ma^2 + 1 \right) \]  \hspace{1cm} (2.78)
By means of this equation it can be shown that it is necessary to use a pressure quotient of at least

\[
\frac{p^*}{p_t} \left( Ma^* = 1 \right) = 0.528
\]  

(2.79)

to operate a convergent-divergent nozzle with air ideal gas ($\kappa = 1.4$) in the supersonic outlet regime. To achieve this, Mach number 1 must be reached at the throat (i.e. throat values are superscripted $^\ast$).

Depending on the relationship between nozzle’s exit pressure and ambient pressure, various jet states can develop, which are shown schematically in Fig. 2.8.

These possible jet formations are listed below and those are classified by their jet-edge shaping, shock-pattern and by the formation of expansion and compression waves:

- (1) convergent-divergent nozzle - $p_e < p_a$ - overexpanded jet
- (2) convergent-divergent nozzle - $p_e > p_a$ - underexpanded jet
- (3) convergent nozzle - $p_e = p_a$ - subsonic jet
- (4) convergent nozzle - $p_e > p_a$ - underexpanded jet
Shocks are defined as infinitesimally thin and discontinuous areas over which flow properties change rapidly and the flow expands from supersonic (i.e. before shock, index 1) to subsonic regime (i.e. after shock, index 2):

\[ Ma_1 > 1 > Ma_2 \]  \hspace{1cm} (2.80)

This situation cannot be treated as isentropic, because entropy increases significantly across the shock

\[ \frac{\partial s}{\partial x} \bigg|_{\text{shock}} \gg 0. \]  \hspace{1cm} (2.81)

Assuming air to be an ideal gas and utilizing the basic Hugoniot relation for static enthalpy before and after the shock (derivation from momentum and energy balance is shown for example in [177])

\[ h_2 - h_1 = \frac{u_1^2}{2} \cdot \left[ 1 - \left( \frac{\rho_1}{\rho_2} \right)^2 \right] \]  \hspace{1cm} (2.82)

relations of flow properties before and after the shock can be written:

\[ \frac{\phi_2}{\phi_1} = f(Ma_1, \kappa). \]  \hspace{1cm} (2.83)

Post-shock Mach numbers can also be calculated as a function of the above variables.

Flow properties across angular shocks, which can be found for example in expanding jets (see the above discussion of Fig. 2.8), are balanced by Eqn. (2.83) taking into account geometric relations between the shock and the mean flow direction (see Fig. 2.9).
The above relations, Eqn. (2.83), are valid in the normal direction across the shock and hence the shock-angle $\Theta$ must be considered in the balancing procedure. The appropriate Mach number to be used in the above relations must be calculated from the velocity component in the normal direction to the shock (superscripted $\{n\}$):

$$Ma_1^{[n]} = \frac{u_1^{[n]}}{a_1} = Ma_1 \cdot \sin(\Theta)$$

so Eqn. (2.83) relations can be modified considering the shock angle

$$\frac{\phi_2}{\phi_1} = f(Ma_1, \kappa, \Theta).$$

Shocks are reflected at solid walls and jet-edges as it is shown in Fig. 2.8.

The non-adiabatic behaviour of particle laden flows inside nozzles is not considered in this work. It is assumed that energy transfer from air to dry-ice particles (which are colder compared to the surrounding air) is negligible inside the short nozzles investigated. However, an assumption is presented in section 4.4.1 for the estimation of a modified nozzle-inlet temperature assuming that there is a considerable cooling effect of the particles upon the air flow during transportation of the particles from the blasting machine to the nozzle through a long tube.
Because modified flow properties influence particle transportation behaviour, these thermodynamic relations must be considered in the particle acceleration simulations presented in this work. The influence of heating or cooling on Mach number is shown in Fig. 2.10.

The curve presented relates enthalpy

\[ h = \frac{\kappa}{\kappa - 1} \cdot \left( \frac{p}{\rho} \right) \]  

(2.86)

to entropy

\[ s = s_0 + c_v \cdot \ln \left[ \frac{p}{p_0} \cdot \left( \frac{\rho}{\rho_0} \right)^{-\kappa} \right] \]  

(2.87)

applying Mach number as curve parameter. Obviously cooling \((q < 0)\) lowers entropy, enthalpy and Mach number in the subsonic regime and increases the latter in the supersonic regime. The non-adiabatic approximations used in this work influence the subsonic regimes only.
Relevance for this work

Dispersed particle phase transport action in compressible air flows is considered by means of source terms in the momentum-balance equations, which is discussed above in section 2.1.2. Particle influence upon turbulence modelling is neglected. Possible interaction effects of finite particles and compressible flow features are addressed in section 4.5 because it turned out to be necessary to improve the drag coefficient formulation used in the numerical code. Non-adiabatic effects are captured by an approximation procedure and this is discussed in detail in section 4.4.

2.3 Axial aircraft compressor aerodynamics

Axial compressors of commercial aircraft engines increase air flow static pressure before it enters the combustion chamber. Modern engines usually have multiple compressors for various pressure levels. Each of these compressor sections consists of numerous stages and each stage comprises a rotor row (i.e. rotating airfoils) and a stator row (i.e. stationary airfoils). Hochschule Darmstadt’s test engine, a GE CF6-50E2, which is investigated in the application study in Chapter 8, has a low- and a high-pressure compressor (LPC and HPC). The low pressure part consists of three and the high pressure part of 14 stages. A section view of this engine is shown in Fig. 2.11.

The desired pressure rise is achieved by convergent-divergent design of the stream channels between the airfoils and by the mechanical work contribution from rotors. The divergent parts of the stream channels are designed to be subsonic diffusers (details described in section 2.2) decelerating the air flow and increasing its static pressure. To understand the main physical phenomena underpinning the influence of airfoil fouling upon compressor performance, it is necessary to introduce some basic values for compressor performance assessment. Figure 2.12 shows a 2D section view of a normalized compressor stage consisting of a rotor and a stator followed by the rotor of the next stage.
Figure 2.11.: GE CF6-50E2 test-engine: section view, LPC and HPC highlighted, drawing from [60].

Figure 2.12.: Characteristic velocity values in representative normalized compressor stage, variables and indexes explained in Tab. 2.9.
Characteristic flow velocities and angles are displayed at the rotor inlet area (1), the intermediate area between rotor and stator (2) and the stator outlet area (3) which is the rotor inlet area (1) of the adjacent compressor stage. Table 2.9 declares all variables and indexes used in Fig. 2.12.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Nomenclature</th>
<th>Index</th>
<th>Nomenclature</th>
</tr>
</thead>
<tbody>
<tr>
<td>$w$</td>
<td>velocity in relative coordinates</td>
<td>1</td>
<td>rotor inlet</td>
</tr>
<tr>
<td>$c$</td>
<td>velocity in absolute coordinates</td>
<td>2</td>
<td>rotor outlet - stator inlet</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>absolute velocity angle</td>
<td>3</td>
<td>stator outlet - rotor inlet</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>ax</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>axial</td>
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<td></td>
<td></td>
<td></td>
<td>rot</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>rotational</td>
</tr>
</tbody>
</table>

Table 2.9.: Variables and indexes used in Fig. 2.12.

By means of total pressure

$$p_t = p + \frac{\rho}{2} \cdot w^2$$  \hfill (2.88)

and corresponding total temperature

$$T_t = T + \frac{w^2}{2 \cdot c_p}$$  \hfill (2.89)

compressor stage pressure ratio

$$\pi_i = \frac{p_{t,3}}{p_{t,1}}$$  \hfill (2.90)

and temperature ratio

$$\tau_i = \frac{T_{t,3}}{T_{t,1}}$$  \hfill (2.91)

are defined and the index $i$ declares a certain compressor stage.
The definition of the specific work of a compressor stage

\[ w_i = c_p \cdot (T_{t,3,i} - T_{t,1,i}) \]  
(2.92)

is used to express the stage's isentropic efficiency

\[ \eta_i^{[s]} = \frac{c_p \cdot (T_{t,3,i}^{[s]} - T_{t,1,i})}{c_p \cdot (T_{t,3,i} - T_{t,1,i})} = \left( \frac{T_{t,3,i}^{[s]}}{T_{t,1,i}} - 1 \right), \]  
(2.93)

which relates isentropic stage work to polytropic stage work.

This expression can be rearranged using the isentropic relationship between total temperature and total pressure ratios

\[ \frac{T_{t,3,i}^{[s]}}{T_{t,1,i}} = \left( \frac{P_{t,3,i}}{P_{t,1,i}} \right)^{\frac{k-1}{k}} \]  
(2.94)

and hence, using Eqn. (2.90), (2.91) and (2.94) in Eqn. (2.93), the isentropic efficiency of a compressor stage can be written

\[ \eta_i^{[s]} = \frac{\tau_i^{\frac{k-1}{k}} - 1}{\tau_i - 1}. \]  
(2.95)

More precise efficiency values can be assessed when using infinitesimal differences instead of stage or even total compressor work values in Eqn. (2.93) resulting in the polytropic efficiency definition:

\[ \eta_i = \frac{dW_i^{[s]}}{dw_i} = \frac{\ln \left( \frac{\tau_i^{\frac{k-1}{k}}}{\tau_i} \right)}{\ln (\tau_i)}. \]  
(2.96)

The derivation of this value from isentropic efficiency by differentiation of the corresponding specific work definitions can be found for example in [24].
By means of reduced mass flux

\[ \dot{m}_{\text{red}} = \dot{m} \cdot \frac{p_{\text{ref}}}{p_{t,\text{IN}}} \cdot \left( \frac{T_{t,\text{IN}}}{T_{\text{ref}}} \right)^{\frac{1}{2}} \]  \quad (2.97)

with

\[ \dot{m} = \rho_i \cdot c_{\text{ax},i} \cdot A_i \]  \quad (2.98)

and reduced rotational frequency

\[ n_{\text{red}} = n \cdot \left( \frac{T_{\text{ref}}}{T_{t,\text{IN}}} \right)^{\frac{1}{2}} \]  \quad (2.99)

compressor performance maps can be drawn, which display compressor pressure ratio as a function of reduced mass flux and which incorporate various parameters such as reduced rotational speed. The above reduced values are normalized to reference ambient conditions

\[ p_{\text{ref}} = 101,325 \, \text{Pa}; \quad T_{\text{ref}} = 288.15 \, \text{K} \]

to make experimental performance mapping comparable and independent from ambient conditions.

An example of such a compressor mapping is shown in Fig. 2.13. The reduction of mass flux at constant rotational speed \( (n_i) \) increases the pressure ratio until the stall curve is reached (upper boundary), where single compressor airfoils begin to stall. Vice versa, reduction of pressure ratio at constant rotational speed increases mass flux until the surge curve is reached (lower boundary) describing the maximum possible flow rate of the compressor.
Figure 2.13.: Typical compressor performance map, original diagram from [24] with modifications.

The dash-dotted line between these margins represents the steady state operational curve. An important design value for the operational point (OP in Fig. 2.13) of compressors is its distance to the stall curve, which represents a safety criterion.

The effect of divergent channel design of any compressor row can be quantified by means of the DeHaller criterion [24, 159]

\[
dH_{rot} = \frac{w_2}{w_1} \quad \text{and} \quad dH_{stat} = \frac{c_3}{c_2}
\]  

which accounts for the possible diffusion of air flow in a particular stage.

If hub or shroud boundary layers are affected by fouling layers, this situation is indicated by \(dH_i\), which tends to increase if aerodynamic blockage of the passage of an airfoil row begins. This blockage effect minimizes the diffusion, because the passage is geometrically modified (i.e. narrowed).
The diffusion number is introduced to additionally account for comparable boundary layer effects at the suction sides of airfoils in a row. It determines a rotor or stator passage loading situation:

\[
D_{f_{rot}} = \frac{w_{max} - w_2}{w_1}; \quad D_{f_{rot}} = \frac{c_{max} - c_3}{c_2} .
\]  (2.101)

The diffusion number represents a modified DeHaller criterion considering the maximum deceleration in the stream channel instead of the total row deceleration of the flow. This diffusion number can be estimated in practical cases as follows according to [24, 159]:

\[
D_{f_{rot}} = 1 - dH_{rot} + \left( \frac{\delta w_{rot}}{2 \cdot \delta l \cdot w_1} \right)_{1-2}; \quad D_{f_{stat}} = 1 - dH_{stat} + \left( \frac{\delta w_{rot}}{2 \cdot \delta l \cdot c_2} \right)_{2-3} \quad (2.102)
\]

where the original DeHaller criterion from Eqn. (2.100) as well as a row loading criterion (see for example [24]) are combined. This loading criterion applies the airfoil’s chord length \( \delta l \) and the spacing between the airfoils \( \delta n \). Furthermore, the maximum deceleration of the row is used and it can be assessed by a relation of the absolute rotational velocity components presented in Fig. 2.12 as follows:

\[
\delta w_{rot} \big|_{i \rightarrow j} = w_{j,rot} - w_{i,rot} = c_j \cdot \sin \left( 90^\circ - \alpha_j \right) - c_i \cdot \sin \left( 90^\circ - \alpha_i \right) .
\]  (2.103)

General methods are discussed in section 2.1 to classify fluid flow states, and the dimensionless numbers presented, such as the Mach and Reynolds number, can be used to classify compressor flows. Flow turbulence and boundary layers are discussed in section 2.1.1.
Referring to these basics, Fig. 2.14 shows a typical flow pattern and boundary layer development across an airfoil. A laminar boundary layer (BL) develops downstream of the airfoil's leading edge until reaching the transition point on either side. This situation is comparable to the boundary layer development over a flat plate, which is discussed in Fig. 2.2.

Transition from laminar to turbulent boundary layer is usually triggered by the beginning of the divergent section of the stream channel in compressor rows and corresponding increasing pressure and decreasing velocity values. Depending on the flow conditions the position of the transition point can change. It is also possible that the boundary layer detaches, which may result in a stall situation and strong passage blockage.

In the case of transonic compressor stages (i.e. incoming flow is supersonic) the convergent part of the stream channel acts to decelerate the flow and shocks can establish, transferring the flow from the supersonic to the subsonic regime (discussed in section 2.2). Shocks are also produced if the incoming supersonic flow hits the airfoil's leading edge. Such a shock can affect the boundary layer negatively, causing thickening or, if the shock is strong, detachment.
Relevance for this work

Summarizing the above, the most important criteria to assess compressor degradation caused by airfoil fouling to be considered in this work are:

• efficiency - $\eta$
• mass flux - $\dot{m}$
• pressure ratio - $\pi$
• DeHaller criterion - $dH$
• diffusion number - $Df$

and these are used to highlight the most important findings from various studies on fouling induced compressor degradation in Chapter 3.

From the relations given above it is clear that compressor performance is strongly influenced by airfoil, hub and shroud surface modifications, for example caused by fouling. These surface modifications from fouling layers can increase the thickness or the roughness (or both). Negative effects of such surface modifications to compressor performance result from boundary layer and stream channel modifications, as is explained above. Their impact is mainly dependent on the main flow state.
3 State of the art

An initial literature survey into axial compressor fouling and cleaning is given in section 3.1. It presents fouling assessment studies and commonly used cleaning methods focussing on aero-derivative engines and stationary gas-turbines. Negative effects of compressor fouling are described and highlighted based on the physical basics given in Chapter 2, section 2.3.

Following this general introduction, the three main research areas of this work are surveyed in detail. These are: precise investigations into dry-ice injection systems in section 3.2 (considered in detail in Chapter 4), particle breakup modelling in section 3.3 (considered in detail in Chapter 5) and defouling erosion modelling in section 3.4 (considered in detail in Chapter 6).

Studies dealing with conventional dry-ice blasting are also considered in this literature survey. Those from KRIEG [103], REDEKER [156] and HABERLAND [72] (all in German) are most important to this work. They contain information on all topics discussed below.

3.1 Axial compressor fouling and cleaning

The literature survey presented in this section provides an overview of axial compressor fouling and cleaning studies. Its main purpose is to guide the reader towards core research topics of this work (see section 1.2). Few studies dealing with aircraft compressor fouling or cleaning can be found in the literature to date, so the survey was extended to include stationary gas turbines.

Compressor fouling was reported to be the main contributing factor to efficiency losses causing as much as 70 to 85% of an engine’s (or gas-turbine’s) efficiency decrease [44, 114, 116, 117, 118, 131, 139]. Fouling was found to be caused by in-service ingestion and deposition of various particles from ambient air, such as salt, unburned hydrocarbons, ash, smog, minerals, insects, oil,
grease, smoke, rust, fertilizers, sand etc. [27, 28, 104, 105, 116, 117, 118, 130]. The probability of deposition depends on particle size and angle of impact upon the compressor’s blading [27, 105]. Atmospheric humidity and ambient temperature were reported to increase the probability of particle deposition [44, 105, 116, 117, 118], because condensed water serves as an adhesive.

**Global effects of fouling**

The accumulated fouling layer was found to add thickness and roughness to compressor airfoils, which decreases mass flux, pressure ratio, efficiency and power output. Furthermore, it narrows the engine’s surge margin [17].

Mass flux is affected by thickened boundary layers and consequent blockage and passage narrowing effects and this influences the surge margin negatively [5, 17, 127, 128, 183]. If a passage is narrowed, its diffusive efficiency decreases and the velocity ratio between inlet and outlet changes and consequently the change in swirl velocity causes a decrease of total pressure ratio [14, 183]. An altered stream channel changes the general flow state, which may trigger some undesired effects upon the main flow features, such as changes to the turbulence regime and as a consequence additional pressure losses and entropy increase [166].

Added airfoil roughness causes repositioning of the transition point of the boundary layer and consequent additional passage blockage, pressure losses and entropy increase. These effects are triggered by earlier development of a turbulent boundary layer [14, 183]. This consumes more of the energy of the main flow and the redirection of the flow in rotor rows may be negatively affected.

In the worst case the boundary layer may detach and the passage may stall. Additional turbulence negatively affects the pressure ratio (i.e. higher pressure losses) and increases the temperature ratio of the stage (i.e. higher tangential stresses, more frictional losses). Both effects decrease the engine’s efficiency.
If constant thrust is to be maintained with a fouled engine, fuel mass flux must therefore be increased to overcome the additional losses and consequently the exhaust gas temperature (EGT) increases. Hence hot-path component creep and engine emissions also increase and this is reported in [38, 44, 104, 117, 118, 131, 132, 133, 134, 183, 188, 189].

**Deposition of fouling**

Front compressor stages were reported to be more prone to fouling deposition compared to rear stages [116, 117, 118, 131, 187, 189], because the freshly ingested ambient air contains the most potential foulants. The leading edges of the blading were found to be most sensitive to fouling, followed by the pressure sides and the suction sides [188, 189].

The leading edges are the first to come into contact with contaminated air and the probability of particle contact with the surface is very high because there is almost no aerodynamic resistance to overcome by the mostly perpendicularly impacting particles.

Contaminants are directed towards airfoil surfaces at concave shaped pressure sides, which makes impacts more possible, and they are redirected from convex shaped suction sides which minimizes the probability of impact and adhesion. In contrast, higher fouling contamination was reported in [149] at the suction

![Image](image.png)

**Figure 3.1.:** Typical turbine airfoil contamination from very small contaminants (i.e. particle diameters smaller than 1 \( \mu m \)) [149].
sides of turbine blades towards the trailing edges compared to lower contaminations at the pressure sides if very small contaminants are considered (i.e. particle diameters lower than 1 µm).

A typical result from this study is shown in Fig. 3.1. Changes in air mass flow rate mainly influence the deposition locations because the air transports the contaminants into the engine and its velocity affects the incident angles of the flow onto the blading (i.e. axial velocity) [105].

Local effects of fouling

The effects on compressor behaviour depend on the location of deposition. Rotor stages were found to be more sensitive to fouling than stator stages and fouled rotor suction sides were found to more negatively affect the overall efficiency compared to fouled pressure sides [5, 127, 128, 183]. This is explainable by consideration of the diffusion effect of a compressor passage, which mainly influences pressure rise and which is mainly influenced by the design of the suction sides. The air velocity is highest at the suction sides and therefore it dominates the friction losses of the passage.

Furthermore, fouled rotors add less rotational velocity to the flow, which may influence a stage’s diffusive efficiency. The rotor’s leading edge and 50% of the suction side chord length were reported to have most influence on the overall efficiency [5, 127, 128, 183], because this region mainly influences the development of the suction side’s boundary layer. These boundary layer changes trigger negative effects such as passage narrowing and diffusion changes.

The decrease in pressure ratio and efficiency was reported to be most significant at normal operational modes hence the airfoils show highest diffusive efficiency at design point (i.e. normal mode) [104, 183]. Effects of altered mass flow rates could also be observed at abnormal operational conditions [104, 183]. Numerous studies presented “intake-depression” as the most important variable.
for in service detection of compressor fouling [44, 116, 117, 118, 131, 188, 189]. It can be defined as follows:

$$\delta p_{IN} := \frac{p_{t,IN} - p_{s,IN}}{p_{t,IN}}$$

(3.1)

with total pressure $p_t$ and static pressure $p_s$ at the throat position of the engine’s intake (index: $IN$). The intake depression accounts for the velocity and consequently for the mass flow into the engine. It decreases significantly if the compressor is fouled and it is measurable in various operational conditions [169].

MOIRINI et al. and ALDI et al. [5, 127, 128] extensively investigated the effects of fouling layers in the NASA Rotor 37 using a number of numerical simulations with Ansys CFX. Various roughness combinations revealed rotor suction sides to be the most important contributors to fouling induced losses. The mass flow rate effect discussed above was reported to be dominant compared to the pressure ratio effect. The authors compared their results to experimental and numerical results reported by SUDER et al. [183] and validated their model. Comparable trends were found and underpredictions from numerical simulations reported in [183] were overcome with the revised modelling strategy presented in [5, 127, 128].

**Defouling**

To counteract the negative effects of compressor fouling, periodical compressor washing is indicated (see for example [131]). As already mentioned in section 1.1, water-wash systems are the current state of the art for aircraft compressor washing. Some studies dealing with parametrization and optimization of such water-based systems can be found in literature [4, 28, 52, 130, 131, 139, 186, 187, 188]. Cleaning agent mass flow rate and droplet diameter were reported to be the main contributing factors to successful online washing of compressors [4, 186, 187, 188]. Most of the cleaning effect was observed shortly after the first injection of cleaning agents, therefore cycle time can be kept to a minimum [4, 28, 130, 186, 187, 188].
The main effect of defouling was found to be mechanical erosion caused by droplet (or particle) impacts on fouled airfoils. The cleaning process is therefore mostly independent from possible additional effects of the medium used according to [28, 130]. Based on [130] and [131] there is an optimum droplet diameter, velocity and spatial distribution to be found and maintained for each individual cleaning case, as long as operational engine parameters remain stable.

Cleaning proves to be insensitive to water temperature, therefore pre-heating was stated to have no beneficial effect in [52, 131]. The main disadvantages of water-based cleaning systems were reported to be the threat of icing (without usage of anti-icing additives) [117, 139] and the risk of redeposition of defouled contaminant particles from front stages at rear compressor stages. Viscous wash agents such as water behave as adhesives [28, 187, 188].

SYVERUD et al. [186, 187, 188, 189] performed salt water deterioration tests on a GE J85-13 jet engine test-rig at various operational modes. The engine was reconditioned by online water-washing (i.e. during engine operation) and performance analysis was reported for a range of compressor conditions and operating points. Fouling locations were found mainly on leading edges and pressure sides; stator rows were more affected than rotor rows and most fouling depositions were found in front compressor stages.

Suction sides of blades contained smaller salt grains compared to pressure sides. Engine recovery was found to be affected by the wash process parameters, with high cleaning mass fluxes and large water droplets cleaning the engine most efficiently. In contrast, lower mass fluxes and smaller droplets caused fouling redeposition at rear stages. Washing efficiency was found to be independent of cycle time.

MEHER-HOMJI et al. [116, 117, 118] published extensive reviews of compressor fouling and cleaning. They classified deterioration parameters and effects as well as typical foulants, as discussed above, and cleaning methods. The sensitivity of front compressor stages to fouling was highlighted. In [116] an original fouling classification map was presented and the authors found original fouling to be a heterogeneous mixture of various particle materials. In
the above authors distinguished recoverable from non-recoverable deterioration and reported compressor cleaning of aero-derivative engines to be of high importance for the operators because up to 20% of the compressor deterioration may be caused by fouling.

KURZ and BRUN gave a comparable overview of compressor fouling and cleaning [104, 105]. They studied the fouling particle behaviour inside compressors in detail and developed and validated a fouling prediction model to be used in conjunction with CFD simulations in BRUN et al. [27]. Furthermore, they studied fouling compositions which can be typically found in axial compressors and created an artificial fouling [28]. With this “dirt formula”, the authors tested the effect of a range of cleaning media upon defouling efficiency and found it to be independent of the medium used. All viscous media considered were, however, prone to trigger redeposition of fouling.

MUND and PILLIDIS [130] investigated water-wash system parameters of a stationary gas turbine intake and discussed air mass flux and droplet diameter, velocity, injection angle and spatial distribution of the droplets using Ansys FLUENT. The main goal of the study was to find a setting which provides a uniform droplet distribution at the compressor inlet. The authors found air mass flux to be sensitive to the washing procedure and suggested to search for optimum parameters of wash-systems for individual (i.e. problem specific) wash-operation conditions.

ENGDAR et al. [52] investigated off-line water-wash injection paths through the bellmouth of a stationary Siemens GTx100 gas turbine by means of the FVM-based CFD code Star-Cd. Boundary conditions for droplet injection (i.e. diameters and velocities) were taken from experiments. Initial water temperature was found to have negligible influence upon the results and predicted wetting of the machine’s IGVs was found to be qualitatively comparable to experimental data.

GILJOHANN et al. [61] reported Euler-Lagrange simulations with Ansys CFX of a preliminary CO$_2$ dry-ice cleaning study of an aero-derivative test engine, type GE CF6-50E2. The particle paths through the engine compressors were dis-
cussed and the particles mainly impacted upon the leading edges and pressure sides of the blading.

Defouling predictions from standard erosion models were qualitatively compared to experimental data but showed unsatisfactory agreement. The necessary future work to overcome the simulation procedure’s weaknesses, which was partially identified in [61], is presented in this study.

### 3.2 Dry-ice injection systems

A detailed investigation of flow pattern and its effect upon particle parameters is required to provide a deeper understanding of particle injection systems (i.e. dry-ice blasting systems) used to clean axial aircraft compressors. Important system parameters, such as system pressure and nozzle type, directly influence particle size distributions and particle velocities entering the aircraft engine.

Blasting systems have been described in a general way by numerous authors [46, 47, 59, 72, 98, 103, 156, 180, 197]. KARPUSCHEWSKI et al. [98] investigated $H_2O$ wet-ice blasting in deburring applications. Sensitive surface blasting was addressed by UHLMANN et al. [197] in the context of injection mould cleaning with $CO_2$ dry-ice snow. DONG et al. [46, 47] used dry-ice blasting systems for the preparation of adhesive surfaces in the context of plasma spraying.

KRIEG (in German) [103] investigated in detail mechanical, thermal and phase-change effects of dry-ice contacts with solid surfaces. He considered conventional dry-ice blasting systems and his main goal was the assessment of defouling.

REDEKER (in German) [156] investigated dry-ice interaction with various targets and focussed a part of his work on substrate and coating erosion. He reported distinct defouling mechanisms and introduced a contact time model for dry-ice particles impacting solid surfaces.
HABERLAND (in German) [72] investigated the conventional dry-ice blasting procedure using theoretical explanations and experimental assessment of erosive and disintegrative mechanisms of impacting dry-ice particles. He estimated thermal stresses for particle-wall contacts.

STRATFORD [180] gave an overview of conventional dry-ice blasting. He highlighted the most significant challenge of experimental dry-ice laden jet investigations to be variable pellet characteristics such as non-uniform shape and size, disintegration and possible particle rotation. Additionally, small sized dispersed dry-ice particles are mostly found to be covered by clouds of CO$_2$ gas and dust in the jets [180].

**Experiments**

Experimental investigations of particle laden jets, comparable to those addressed in this work, are presented in [54, 72, 110, 156, 157, 176, 198, 205] and methods and variables used in these studies are listed in Tab. 3.1 and discussed below.

LIU et al. [110] investigated dry-ice particle agglomerations in a rapid expansion nozzle for liquid CO$_2$. Particle re-entrainment from accumulated wall-layers was identified as a main agglomeration mechanism. The jets investigated were consequently laden with CO$_2$ snow. LIU et al. utilized Laser Doppler Measurement (LDM) to determine particle sizes exiting all nozzles investigated. They found particle sizes decreasing with increasing jet velocity.

FAN et al. [54] presented particle image velocimetry (PIV) experiments of micro-abrasive jets. They used a laser exposure system to visualise particles made from Aluminum (Al) and found particle velocity to be a function of system pressure and axial distance from the nozzle exit. The variation of particle velocity was up to 80 m/s for constant system settings.

UHLMANN et al. presented a new acceleration system for dry-ice particles in [198] and investigated particle velocities by means of a high-speed camera system (HSC).
### Table 3.1:
Comparison of methods and variables from experimental investigations of particle laden jets from literature.

<table>
<thead>
<tr>
<th>Study</th>
<th>Experimental method</th>
<th>Particle material</th>
<th>Range of particle diameters [$\mu m$]</th>
<th>Range of particle velocities[$m/s$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAN et al. [54]</td>
<td>PIV (HSC)</td>
<td>Al</td>
<td>27</td>
<td>40 - 150</td>
</tr>
<tr>
<td>HABERLAND [72]</td>
<td>PIV (HSC)</td>
<td>dry-ice</td>
<td>400 - 1000</td>
<td>110 - 275</td>
</tr>
<tr>
<td>LIU et al. [110]</td>
<td>LDM</td>
<td>dry-ice</td>
<td>1 - 100</td>
<td>n.a.</td>
</tr>
<tr>
<td>REDEKER [156]</td>
<td>PIV (HSC)</td>
<td>dry-ice</td>
<td>ca. 100 - 3000</td>
<td>150 - 450</td>
</tr>
<tr>
<td>REDEKER et al. [157]</td>
<td>PIV (HSC)</td>
<td>dry-ice</td>
<td>ca. 100 - 3000</td>
<td>175 - 400</td>
</tr>
<tr>
<td>SPUR et al. [176]</td>
<td>PIV (HSC)</td>
<td>dry-ice</td>
<td>1000 - 3000</td>
<td>120 - 280</td>
</tr>
<tr>
<td>UHLMANN et al. [198]</td>
<td>PTV (HSC)</td>
<td>dry-ice</td>
<td>n.a.</td>
<td>8 - 70</td>
</tr>
<tr>
<td>WESTON et al. [205]</td>
<td>MV</td>
<td>dry-ice</td>
<td>ca. 500</td>
<td>155 - 241</td>
</tr>
</tbody>
</table>

REDEKER et al. [157] presented particle sizes and velocities from HSC investigations of dry-ice blasting nozzles for a range of operational parameters. A later work by REDEKER [156] contains additional experimental data. Comparable HSC experiments were also presented by SPUR et al. [176] and HABERLAND [72].

KRIEG [103] used the velocity correlation presented by SPUR et al. [176] to predict dry-ice particle exit velocity for his basic studies of dry-ice cleaning mechanisms mentioned above, however he stated that particle diameters and velocities were strongly dependent on system parameters.

WESTON et al. [205] used a mechanical velocimeter (MV) to estimate dry-ice particle velocities in polymer substrate decoating experiments. The relationship between particle velocity and system pressure was calibrated using experimental data.

A significantly larger minimum particle diameter was found by SPUR et al. [176] compared to the other studies and significantly higher maximum velocities are encountered in the outcomes from REDEKER et al. [156, 157] compared to the others. The most frequently used method to size and track particles from accelerating blasting nozzles is HSC based PIV.
LONGMIRE and EATON [111] presented a more fundamental study of particle laden jets. The authors carried out laser-illuminated recordings for particle visualization and used LDM to estimate particle velocities. The study was focussed on solid particles with Stokes numbers around unity and subsonic flow. These particles were prone to be clustered by vortex structures in the jets and the authors found significantly non-uniform particle concentrations. The jets were therefore reported to be highly discontinuous and time-dependent, which was stated to have been neglected in time-averaged former studies of comparable situations.

**Simulations**

Numerical simulation of particle laden compressible flows though convergent-divergent nozzles was addressed by various research groups. DONG et al. supported their work mentioned above [46, 47] by means of a numerical Euler-Lagrange investigation of dry-ice blasting nozzles with Ansys CFX and this is reported in [48].

In this study the acceleration of dry-ice particles was considered as a function of system and particle parameters. The authors optimized the nozzle geometry of the related application. Particle sizes were assumed to be constant, and only the particle mass flow rate and the particle shape factor were parametrized.

POUGATCH et al. [152] investigated gas-assisted atomization with an Euler-Euler approach using Ansys Fluent. The utilization of a virtual mass contribution in the conservation equations of the particle phase was necessary due to a high gas-volume fraction. The numerical results were partially compared to experiments which showed good agreement.

In a later work, POUGATCH et al. [153] investigated supersonic nozzles for particle agglomerate attrition to avoid growing agglomerates in a fluidized bed system. They used an Euler-Euler approach and considered interfacial heat transfer to optimize attrition efficiency by varying a number of system parameters.

ADAMOPOULOS and PETROPAKIS [2] investigated dissociation and distribution of dispersed droplets in supersonic ejector geometries used in food applic-
ations. The authors optimized the geometry involved and investigated the flow in detail. Special attention was paid to turbulent dilation dissipation at high Mach numbers. It was shown that the droplet distribution and possible pasteurization effects of the droplets can be triggered by an optimized geometry influencing the supersonic flow and its interaction with the droplets.

YIN et al. [209] reported a numerical study of cold spraying applications. They simulated the acceleration of copper particles in a 2D Euler-Lagrange formulation through a convergent-divergent nozzle and discussed the optimum expansion ratio of the nozzle as well as the acceleration behaviour of the particles. They found particle velocities to be dependent on particle size, system pressure and nozzle length. An optimum length was found for a set of constant system parameters.

Particle transport is numerically modelled by means of an Euler-Lagrange particle tracking formulation in this work. Focussing on dispersion and turbulent motion prediction, GOUESBET and BERLEMONT [65] gave a detailed overview of the general methods to simulate such phenomena. They discussed coupling techniques as well as Euler-Euler and Euler-Lagrange methods. The development of the basic Lagrangian formulation for a non-rotating particle was reviewed in the context of various constraints regarding forces consideration in [65]. The necessity of modifications of the momentum and turbulence equations of the continuous phase triggered by the dispersed phase was highlighted, if 2-way coupling was indicated. In this case fluid reactions to particle acceleration must be considered.

LAIN and SOMMERFELD [106] presented 2-way and 4-way coupling methods for the simulation of horizontal channel conveying. Particle-fluid and particle-particle interactions were considered for prediction of the dispersed particle trajectories and this was called the 4-way coupling method. An overview of Euler-Euler and Euler-Lagrange methods and a turbulence model discussion was given in reference [106]. The turbulence models considered in [106] were modified in the 2-way and 4-way coupling schemes by means of source terms.

ELGOBASHI [50] presented a particle laden flow classification map dealing with the interaction of dispersed particles with turbulent structures. He also
gave an overview of the above Euler-Euler and Euler-Lagrange methods. He proposed a preliminary investigation of the number of model particles to be considered for Euler-Lagrange simulations and a statistical formulation of the local particle number simulated. The latter might be used to account for the clustering and non-uniform particle behaviour discussed above in LONGMIRE and EATON [111]. The outcomes from [50] are only valid for incompressible, isothermal flows without phase-change. In a later work [51], ELGOBASHI updated his classification map based on detailed direct numerical simulations (DNS). He found the 2-way coupling regime to be turbulence enhancing or dissipating depending on turbulent Stokes numbers.

3.3 Particle breakup modelling

The most important findings from literature related to the development of the particle breakup model presented here are summarized in this section. Since there are only a few phenomenological particle breakup studies published for CO$_2$ dry-ice, publications are considered which deal with materials showing impact and breakup behaviour comparable to what is expected to apply for dry-ice. Examples of such materials are brittle agglomerates, industrial granules and water-ice.

Dry-ice studies

Dry-ice breakup studies have been published by KRIEG [103], REDEKER [156] and HABERLAND [72] who investigated dry-ice particles impacting solid walls with HSC experiments and theoretical approaches. Their findings phenomenologically describe the breakup process.

KRIEG [103] used an overall energy balance of the impacting particles and concluded that impact induced sublimation affects only a negligible proportion of particle mass. However, he claimed that local sublimation is possible due to partial pressure modifications on impact. Material properties for dry-ice are summarized in [103]. According to this, the crystalline density of dry-ice is
1564 kg/m³, however the density of dry-ice pellets is reported to be lower due to gaseous inclusions and production related impurities.

REDEKER [156] also used an overall energy balance to discuss the single energy contributors in detail, which are significant if a particle impinges a wall. He found only a negligible proportion of mass being prone to sublimation upon impact. Following [156], the dry-ice particle breakup process is mainly dependent on impact velocity and particle size. Experiments were made to measure Young’s modulus of a number of artificial dry-ice specimens, which, however, were significantly larger compared to conventional dry-ice pellets used in typical dry-ice blasting applications. Material properties for dry-ice are also summarized in [156] and the actual density of dry-ice pellets is reported to be in the range from 650 to 1050 kg/m³.

HABERLAND [72] used a HSC and found dry-ice particles disintegrating into dust, liquid and a proportion of mass sublimating on impact. However, he calculated, using a basic energy balance of the impacting particle, that a theoretical maximum proportion of 15 % of primary particle mass can sublime upon impact. Furthermore, he reported the actual density of dry-ice pellets to be in the range from 1300 to 1560 kg/m³ influenced by various inclusions. These values are significantly higher compared to those reported by REDEKER in [156]. The most important material properties of dry-ice are listed in Tab. 3.2 below, comprising a summary from literature and comparing the values to water-ice.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density $\rho$ [kg/m³]</th>
<th>Young's modulus $Y$ [GPa]</th>
<th>Heat conductivity $\lambda$ [W/m·K]</th>
<th>Specific heat capacity $c_p$ [J/kg·K]</th>
<th>Phase change enthalpy $\delta h_{pc}$ [J/kg]</th>
<th>Phase change temperature $T_{pc}$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CO_2$ dry-ice</td>
<td>466 - 1560</td>
<td>0.23</td>
<td>0.0164</td>
<td>780 - 850</td>
<td>573,200</td>
<td>-78.5</td>
</tr>
<tr>
<td>$H_2O$ water-ice</td>
<td>920</td>
<td>0.3 - 11.7</td>
<td>2.22</td>
<td>2,000</td>
<td>334,000</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 3.2.: Comparison of $CO_2$ dry-ice and $H_2O$ water-ice properties from literature utilizing data from [62, 72, 87, 103, 119, 156, 168, 201].
Water ice studies

Water-ice breakup studies are more commonly found and provide more detailed insight into ice-particle breakup behaviour upon solid target impacts. The most recent studies are those of VARGAS et al. [200] and HAUK et al. [77, 78].

VARGAS et al. [200] used two HSCs to track and size pre- and post-impact particles. The ice spheres investigated were artificially made by water droplet injection into a sub-cooled fluid. They were accelerated by a gas-gun and impacted a glass plate in the 45° direction over a range of velocities. The authors found a cloud of fines (i.e. very small post-impact particles) occurring directly after impact and discussed various post-processing strategies to detect and size dispersed post-impact particles.

The most effective way to find the dispersed secondary particles in the recordings was waiting until the fast and dense secondary dust-cloud disappeared. The remaining secondary particles were found to be distributed along the impacted surface, moving with almost no normal velocity component to the wall. Therefore the impact process was reported to be quasi 2D. Furthermore, spatial and temporal discretization and the selection of the field of view of the HSCs for setting-up such particle breakup experiments was discussed in detail. Weaknesses of the recordings, such as blurred images due to post-impact dust, camera-lens distortion or shadowing, were also discussed.

HAUK et al. [77, 78] impacted solid targets with single primary particles with various sizes and velocities. The single particle impacts were selected from dilute laden air flow records. One of the goals of the study was to discuss the main fragmentation modes of water-ice and to find a physical formulation for the threshold value between these modes.

HAUK et al. presented a combination of impacting velocity $v_p$, particle diameter $d_p$ and a new parameter $\beta$

$$
\tau_{tr} = \frac{v_p \cdot d_p^2}{\beta}
$$

(3.2)
and it was used to distinguish between the following fragmentation modes defined in [77, 78]:

- no fragmentation
- minor fragmentation
- major fragmentation
- catastrophic fragmentation.

The authors also discussed the normal and the tangential coefficient of restitution of secondary particles

\[ \epsilon_{\text{dir}} = \frac{v_{p_2}^{\text{dir}}}{v_{p_1}^{\text{dir}}} \]  

(3.3)

where the direction is indicated by the superscript \( \text{dir} \). The normal coefficient of restitution and the post-impact angle were reported to decrease with increasing impact velocity and primary particle diameter. The tangential coefficient of restitution was found to be approximately constant and the post-impact angle was found to be dependent on \( \gamma_{trv} \) from Eqn. (3.2).

PAN and RENDER [143, 158] presented experiments comparable to what was reported by VARGAS et al. [200] in previous studies. They measured post-impact particle velocities and sizes from HSC recordings. They also found a densely-laden cloud of post-impact dust moving initially at a higher velocity than the primary particle impact velocity. Velocities of single secondary particles were measured after the cloud of dust disappeared.

GUEGAN et al. [69] utilized the same technique. They tracked secondary particles and found various post-impact velocities ranging from almost stationary particles remaining approximately at the impact point to very fast particles. The latter describe a circular envelope of the post-impact cloud of dispersed particles, which forms after disintegration according to [69, 158, 200].

This cloud-velocity was approximated by PAN and RENDER [143, 158] in 2D along the impacted target as there was almost no bounce (i.e. no normal post-impact velocity) detected. PAN and RENDER also found secondary particle
velocities to be a function of the tangential proportion of impact velocity, which was confirmed by GUEGAN et al. [69]. The latter authors described secondary particle diameters as function of normal impact velocity component.

Numerous authors discussed coefficients of restitution, Eqn. (3.3), for water-ice impacts and agreement can be summarized upon the general functional relation

\[ \varepsilon^{\text{dir}} = f \left( v_p^{\text{dir}}, d_p, \alpha_p, \text{surface} \right) \]  

representing this coefficient as a function of particle impact velocity, diameter, impact angle \( \alpha_p \) and impact surface conditions (frost, coating, macroscopic roughness etc.) [70, 75, 77, 78, 83, 84, 158]. In some studies, the coefficient of restitution was found to be independent of the target temperature [70, 75, 158]. The secondary particle velocity in normal direction was found to be negligible in various studies [69, 77, 78, 143, 158, 200]. Some authors found absolute values of secondary particle velocities ranging from approximately stationary to values higher than the impact velocity [69, 158, 200].

TUHKURI [196] reported fracture mechanisms for water-ice disintegration to be flaking, fragmentation and breaking. VIDAURRE and HALLETT [201] distinguished between no breakup and severe breakup of ice particles typically found in clouds by means of the Weber number

\[ \text{We} = \frac{v_p^2 \cdot d_p \cdot \rho_p}{12 \cdot \sigma} \]  

which includes particle surface tension \( \sigma \) representing its breakage resistance. A functional relationship for the secondary particle diameters \( d_i \), comparable to what is reported above for the coefficient of restitution, can be summarized as follows:

\[ d_i = f \left( v_p, d_p, \alpha_p \right) \]  

and it indicates that the breakup process is mainly a function of impact velocity, primary particle diameter and impact angle [143, 158, 196, 200, 201].
Water-ice properties were reported for example in [62, 87, 119, 168, 201] and the most important findings are summarized in Tab. 3.2 and compared to dry-ice properties, which is discussed above. A typical stress-strain curve for water-ice is shown in Fig. 3.2 according to [41, 119, 168]. It incorporates indicators for first failure nucleation (N) and failure propagation (P) until total fault. This was reported to be typical water-ice behaviour in [41, 119, 168].

Grain size [41, 168], temperature and gaseous or solid inclusions [87] were reported to influence water-ice particle stress resistance. Results comparable to the above water-ice findings were reported by RUSSELL et al. [162] who performed diametral compression tests of various elastic-plastic granules.

The authors found the Young’s modulus of the tested granules to increase with decreasing size and decreasing water content. They discussed onset of granule breakup to be dependent on void fraction, number of bonds, pre-existing flaws and particle diameter.
Granular material studies

Experimental and numerical breakup studies dealing with various granules and agglomerates were reported by numerous authors and the studies most important to this work are summarized below. ANTONYUK et al. [10] investigated representative granules of elastic, elastic-plastic and plastic breakup behaviour. The authors performed static breakup and dynamic impact experiments and concluded that particle breakup behaviour was mainly dependent on diameter and interfacial energy of the primary particles (in this case the small particles being agglomerated to larger particles).

Dynamic impact tests revealed further dependence on impact velocity and angle. These results were confirmed by numerous other experimental and numerical studies [6, 32, 33, 34, 74, 95, 123, 126, 160, 164, 181, 192, 195, 202]. Superficial flaws were found to initialize the breakup process of elastic materials by ANTONYUK et al. [10]. Elastic-plastic particles were found to have disintegrated due to internal bond-fails and plastic granules were found to break up due to propagation of pre-existing flaws.

Compression tests of elastic-plastic material were simulated by means of DEM and these results were compared to the above experiments in [11]. It was shown that bond failure initializes the breakup. A good agreement between experimental and numerical outcomes was found. ANTONYUK et al. [11, 12] reported similarities between static and dynamic breakup behaviour for these granules. This finding can be confirmed by a previous study from SHIPWAY and HUTCHINGS [172].

Failure modes and breakup regimes were investigated in numerous studies dealing with granules and agglomerates, for example in [30, 71, 95, 96, 125, 150, 151, 164, 182, 193, 202]. POPATOV and CAMPBELL [150, 151] distinguished between two breakup mechanisms in their numerical and experimental studies and found these mechanisms to be dependent on impact velocity and wall material. They reported secondary particle diameters to be correlated to low and high impact velocities but in the medium range of impact velocities these diameters were found to be independent from impact velocity.
THRONTON et al. came to comparable conclusions utilizing DEM simulations [96, 125]. They distinguished various failure modes as follows:

- no fracture
- fracture
- shattering
- total disintegration

and stated in [96] that “no fracture” and “shattering” were velocity dependent while the “fracture” mode was found to be bond energy dependent only. THRONTON et al. [96, 125, 181, 192, 193] also subdivided secondary particles into classes dependent of their proportion of mass $m$ related to the primary particle mass $M$ as follows:

- residue ($\frac{m}{M} \geq 0.1$)
- debris ($\frac{m}{M} < 0.1$).

The authors dealt with the proportion of residue and debris produced by the above fragmentation modes in [125] and found the proportion of debris particles increasing by secondary impacts after the actual primary particle impact [193].

Secondary particle sizes were reported to be a function of impact velocity in [30, 32, 33, 34, 123, 160]. A critical velocity for the onset of granule breakage upon impact was investigated in [7, 8, 30, 74, 172] and all authors concluded that critical threshold velocity was a function of primary particle diameter and various material properties, from which internal bond energy was found to be most important.

CARMONA et al. [30] investigated fragmentation regimes of model agglomerates with FEM and DEM simulations and reported fragmentation to be mainly dependent on impact velocity. They found that particles suffer initial internal damage before first cracks could be seen externally. This initial damage was reported to be not experimentally detectable.
Figure 3.3.: Reconstructed spherical agglomerates after DEM breakup simulations with various impact velocities $v_j$ ($j = 1...6$ increasing from upper left to lower right display) adapted from [30].

Figure 3.3 contains images of crack patterns at the surface of simulated agglomerates produced by various impact velocities from [30]. Vertical cracks disintegrated the particle into large secondary fragments at low velocities, while higher impact velocities produced additional lateral cracks, which leads to further disintegration and increasing numbers of smaller sized secondary particles. These findings are comparable to what was reported in some other studies dealing with various granules [96, 125, 182, 192, 193, 202] and also for water-ice [77, 78].

The initial production of very small secondary particles (i.e. “fines”) at primary particle impact described above was also observed in a range of publications dealing with granules [96, 125, 193, 202]. SCHUBERT et al. [202] experimentally observed this phenomenon and investigated it in more detail by means of FEM and DEM based numerical studies for concrete particles. They defined this region as the “cone of fines” and their findings are comparable to findings from the above water-ice studies by HAUk et al. [77, 78].
The Weber number as defined above, Eqn. (3.5), used for classification of water-ice fragmentation modes in [201], was modified by THRONTON et al. [192], SUBERO et al. [181] and MORENO-ATANASIO and GHADIRI [126]

\[
We^* = \frac{(v_p - v_{trv})^2 \cdot d_p \cdot \rho_p}{\gamma_0}
\]  

(3.7)

to express the damage ratio of model granules in various DEM simulations as a function of threshold velocity \(v_{trv}\), which indicates the onset of breakup, and of internal bond energy \(\gamma_0\). However, MORENO-ATANASIO and GHADIRI [126] reported that the damage ratio can only be expressed as a function of this number if the differences of internal energy of various investigated granules are small. They addressed the necessity of further investigations towards a more general expression.

### 3.4 Defouling erosion modelling

The compressor defouling simulations required in this work must incorporate an appropriate erosion prediction formulation and this process must be simulated using Ansys CFX. This code currently incorporates turbomachinery-specific erosion models from FINNIE [56] and GRANT and TABAKOFF [66]. FINNIE [56] analysed basic principles of ductile and solid target material erosion and gave basic relations between erosion rate, particle impact velocity and impact angle. GRANT and TABAKOFF [66] developed a full theoretical approach to predict particle trajectories and rebounding behaviour, as well as erosive action of various particles investigated in turbo-machinery simulations. Neither model is designed to predict coating erosion.

The following literature review comprises various erosion model approaches as well as decoating studies and single particle impact testing. The scope of the review is broad since compressor defouling is not directly comparable to solid material erosion or decoating applications due to the amorphous and heterogeneous nature of the fouling.
**Conventional erosion models**

The literature contains a large number of semi-empirical erosion models. They were mostly developed for particular applications and can be described as follows, where \( ER \) is the predicted amount of erosion:

\[
ER = \prod_i (K_i \cdot v_p^n \cdot d_p^m \cdot F(\alpha_p) \cdot F(\psi)).
\] (3.8)

Typically, such models include a range of material-dependent factors \( K_i \), and power-law expressions for particle velocity \( v_p \) and size \( d_p \). Model constants and exponents must be derived from basic experiments. Some models also include functional relations \( F \) of impact angle \( \alpha \) and material properties (here represented by \( \psi \)). One such model is the Tulsa erosion model [39, 215]. It was developed to predict erosion by dispersed particles in oil pipelines.

A comparable but more general model is that from OKA et al. [137, 138], which can be adapted to various situations with experimental calibration. Another approach is the micro-scale dynamic modelling described by LI et al. in [37, 108], which accounts for mechanical properties of the materials investigated by direct simulation of the material matrix. This method is computationally expensive for large-scale simulations.

**Coating erosion**

Erosion of coatings without substrate penetration has been studied by a number of researchers. A selection of the most relevant studies to this work is listed in Tab. 3.3 and the studies are discussed below.

CERNUSCHI et al. [31] experimentally investigated erosion of thermal barrier coatings (TBC) from hot-path gas turbine components. The authors stated particle kinetic energy to be the most important erosion factor because experimental erosion rates were proportional to the square of the impact velocities. Increased target temperatures increased the erosion rates.

DJUROVIC et al. [45] experimentally investigated organic coating defouling and found particle impact velocity to be most important to total erosion results.
<table>
<thead>
<tr>
<th>Study</th>
<th>Coating</th>
<th>Particles</th>
<th>Type of Study</th>
<th>$d_p$-range [$\mu m$]</th>
<th>$v_p$-range [$m/s$]</th>
<th>main ER contributors</th>
</tr>
</thead>
<tbody>
<tr>
<td>CERNUSCHI et al. [31]</td>
<td>TBC ceramics</td>
<td>$Al_2O_3$</td>
<td>EXP</td>
<td>16.7, 126</td>
<td>60, 104</td>
<td>$v_p$ and $T_{tar}$</td>
</tr>
<tr>
<td>DJUROVIC et al. [45]</td>
<td>organic</td>
<td>wheat-starch</td>
<td>EXP</td>
<td>400, 600, 1100</td>
<td>140 - 250</td>
<td>$d_p$ and $v_p$</td>
</tr>
<tr>
<td>KIM et al. [99]</td>
<td>WC-Ni</td>
<td>$Al_2O_3$</td>
<td>NUM &amp; EXP</td>
<td>50</td>
<td>30</td>
<td>coating hardness</td>
</tr>
<tr>
<td>LI et al. [109]</td>
<td>paint</td>
<td>ceramics</td>
<td>EXP</td>
<td>300 - 900</td>
<td>47 - 116</td>
<td>$d_p$ and $v_p$</td>
</tr>
<tr>
<td>PAPIN and SPELT [146]</td>
<td>polyamide &amp; polyurethane</td>
<td>steel</td>
<td>TRY &amp; EXP</td>
<td>890</td>
<td>55</td>
<td>elastic-plastic processes</td>
</tr>
<tr>
<td>SHIPWAY et al. [173]</td>
<td>paint and chrome</td>
<td>glass</td>
<td>EXP</td>
<td>255</td>
<td>73, 110</td>
<td>cracking, fracture, ...bending, $d_p$ and $v_p$</td>
</tr>
<tr>
<td>ZHANG and DONG [212]</td>
<td>metallic-ceramic-composite</td>
<td>catalyst</td>
<td>NUM</td>
<td>60 - 120</td>
<td>50 - 250</td>
<td>$d_p$ and $v_p$</td>
</tr>
<tr>
<td>ZOUARI and TURATIER [217]</td>
<td>paint</td>
<td>steel, Al, polyacetat</td>
<td>NUM</td>
<td>2000</td>
<td>35 - 200</td>
<td>penetration, buckling, ...delamination and $v_p$</td>
</tr>
</tbody>
</table>

Table 3.3.: Overview of coating erosion studies.
and particle diameter to be most important to the onset of erosion. The latter mainly increased the “damage-per-impact” rate. Furthermore, the authors reported that coating hardness determined maximum erosion rates as a function of impact angle. Harder coatings were removed more efficiently at normal impact conditions and angular impacts were stated to be more favourable for softer coatings.

KIM et al. [99] carried out experiments and numerical investigations towards the predictive capabilities of Ansys CFX, version 11.0. They discussed the influences of turbulence models upon calculated erosion rates on coated substrates from standard erosion models. The most precise predictions were reported with the SST model (see section 2.1.1) and increasing erosion rates were found if coating hardness was increased.

LI et al. [109] also determined particle impact velocity and diameter to be the most important variables influencing erosion rates with experimental single particle investigations. They stated velocity to have less influence compared to diameter.

PAPINI and SPELT [146] investigated elastic-plastic mechanisms of polyamide and polyurethane coatings with single particle impact experiments. They presented approaches for prediction of crater size, shape and rebound of impacting particles as a function of impact velocity and angle. Furthermore, a new method was presented to determine coating dynamic hardness, which was proposed originally by TIRUPATAIAH and SUNDARARAJAN [194] to characterize coating materials by means of impacting particle energy.

SHIPWAY et al. [173] investigated cracking, fracture and bending processes of paint and chrome coatings in erosion experiments. They reported the erosion rate of chrome to be a function of impact kinetic energy.

ZHANG and DONG [212] applied FEM simulations with LS-DYNA to assess metal ceramic composite coating erosion. They discussed stress distribution from coating to substrate as well as kinetic energy effects of the impinging particles and concluded that particle impact velocity and diameter were the most important variables influencing the erosion rate.
ZOUARI and TOURATIER [217] reported detailed investigations into penetration, buckling and delamination mechanism of paint coatings upon indentation. Their study was experimental and numerical and they used the FEM based code LS-DYNA and a Johnson-Cook approach to simulate paint layer erosion by single particle impacts. The authors discussed energy balances of impacting particles as well as buckling and delamination processes and found that increasing impact velocities increased erosion rates.

A summary of the above findings is given in Eqn. (3.9) and it shows the general functional relation between the erosion rate of a coating material and characteristic eroding particle variables

\[
ER = f (d_P, v_p, \alpha_p, \psi)
\]  

(3.9)

and most of these variables are also contained in the above relation for substrate materials, Eqn. (3.8).

**Figure 3.4.** Erosion rate as a function of impact angle for brittle and ductile material with data for brittle SiC and ductile Cu from [37].
Impact velocity was found to be an important contributor to coating erosion in multiple studies [21, 31, 45, 109, 173, 212, 213] and also particle diameter was often found to be very important [21, 45, 109, 173, 174, 207, 212]. A certain influence of the impact angle is also confirmed by many researchers [21, 31, 45, 136, 171, 199, 204] but it depends on the coating material considered.

Furthermore coating material properties, such as ductility, hardness or porosity were also found to be important contributors to decoating erosion by various authors [21, 25, 31, 99, 136, 204]. The brittleness of the penetrated material mainly determines maximum erosion rates and these are a function of the impact angle, which is shown in Fig. 3.4 for typical brittle and ductile materials. Trends comparable to those can be found for example in [37, 56, 66, 88, 108].

**Particle indentation studies**

In order to determine the behaviour of fouling layers on particle impact during engine cleaning, this literature survey was extended to single particle indention studies. Several researchers have taken a single particle assessment approach to investigate indentions into pure materials or coatings in terms of elastic and plastic deformation regimes under consideration of surface forces and their work is summarized in Tab. 3.4 and discussed below.

BARNOCKY and DAVIS [18] and DAVIS et al. [42] experimentally investigated rebound characteristics for single particles made from plastic and metal impacting quartz targets coated with viscous fluids. They discussed the coefficient of restitution for single particles as a function of near wall Stokes number, coating thickness and substrate roughness. The near wall Stokes number was derived from the particles ODE of motion, Eqn. (2.64), in near wall formulation only considering viscous forces (index: c for coating):

\[
St_c = \frac{m_p \cdot v_p}{6 \cdot \pi \cdot \eta_c \cdot r^2_p} = \frac{1}{9} \cdot \frac{\rho_p \cdot v_p \cdot d_p}{\eta_c} \quad (3.10)
\]

The above authors found the viscous coating layer to be responsible for lower restitution coefficients due to higher energy dissipation in certain Stokes num-
<table>
<thead>
<tr>
<th>Study</th>
<th>Coating (C) or Substrate (S)</th>
<th>Particles</th>
<th>Type of Study</th>
<th>$d_p$-range [$\mu m$]</th>
<th>$v_p$-range [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BARNOCKY and DAVIS [18]</td>
<td>C: viscous &amp; rough</td>
<td>steel, acrylic</td>
<td>TRY &amp; EXP</td>
<td>800 - 3200</td>
<td>??</td>
</tr>
<tr>
<td>DAVIS [42]</td>
<td>C: viscous</td>
<td>metal, plastic</td>
<td>TRY &amp; EXP</td>
<td>6400, 9600, 12800</td>
<td>??</td>
</tr>
<tr>
<td>HUTCHINGS et al. [90, 91]</td>
<td>S: mild steel</td>
<td>steel, quartz, WC</td>
<td>TRY &amp; EXP</td>
<td>9500</td>
<td>141 - 400</td>
</tr>
<tr>
<td>KLEIS and HUSSAINOVA [101, 102]</td>
<td>S: lead, copper, aluminum, steel, ceramics</td>
<td>glass, stainless steel</td>
<td>TRY &amp; EXP</td>
<td>700, 1600</td>
<td>20 - 100</td>
</tr>
<tr>
<td>PAPINI and SPELT [145]</td>
<td>C: alkyd</td>
<td>glass</td>
<td>TRY &amp; EXP</td>
<td>640</td>
<td>10 - 120</td>
</tr>
<tr>
<td>SUNDARARAJAN et al. [184, 194]</td>
<td>S: iron, copper</td>
<td>steel, WC</td>
<td>TRY &amp; EXP</td>
<td>4760</td>
<td>5 - 200</td>
</tr>
<tr>
<td>WALL et al. [203]</td>
<td>S: molybdenum, silicon, mica, tedlar</td>
<td>ammonium fluoride</td>
<td>TRY &amp; EXP</td>
<td>2.6 - 6.9</td>
<td>1 - 100</td>
</tr>
</tbody>
</table>

**Table 3.4:** Overview of coating erosion studies.
ber ranges. No difference could be detected between restitution of particles from coated to bare substrates in high Stokes number ranges.

HUTCHINGS et al. [90, 91] investigated restitution properties of single particles made from steel, quartz and tungsten carbide (WC) impacting mild steel targets over a range of velocities and impact angles. The restitution behaviour of these particles was investigated experimentally. Crater volume and dissipated energy (i.e. “crater formation energy”) were found to be functions of impact angle and velocity. Similarity between craters from particles of various material was reported. A crater formation and energy consumption model was generated based on those findings and later it was implemented in software [92].

KLEIS and HUSSAINOVA reported specific crater-formation energy as material constant representing its dynamic hardness, which can be derived from single particle impact experiments and energy-based theory [101, 102]. In further studies [88, 89], this energy-based description was modified by momentum-based impact formulations allowing the calculation of kinetic energy losses. These can be described by restitution and friction coefficients based on the sliding and rolling regime of the impacting particle upon wall contact.

PAPINI and SPELT [145] investigated glass bead impacts against alkyd coated steel substrates to assess coating removal. They measured energy losses and restitution behaviour of impacting particles and developed an energy-based model to predict coating removal. They found coating removal to be independent of tangential forces and reported only the shape of indentation changing with increasing impact angles. Furthermore, they found that the coefficient of restitution can be used to determine energy dissipation over a range of normal impact velocities up to a certain maximum. Coating thickness was found to be negligible in indentation surface estimations. The onset of erosion was related to full penetration of the coating. It was shown in later communications by the authors [147, 148] that the critical energy required to initially penetrate a coating is independent of the particle material and that decoating happens if the impacting particles initially penetrate the coating to the substrate.
SUNDARARAJAN et al. called the above experimental technique presented in [90, 91] "Dynamic Indentation Testing" (DI) and performed comparable experiments with single steel [184] and WC [194] particles impacting ductile target materials with various velocities and impact angles. In [184] an energy-based model was introduced to predict crater volume and particle rebound characteristics. The authors introduced dynamic hardness

\[ H_d := \frac{1}{2} \cdot m_p \cdot \frac{v_{p,1}^2 - v_{p,2}^2}{v_{imp}} = \frac{1}{2} \cdot \frac{m_p}{V_{imp}} \cdot v_{p,1}^2 \cdot (1 - \epsilon^2) \]  

(3.11)
as an important material property which relates dissipated energy of the impacting particle to the volume of the crater formed on impact. They also defined a range of requirements to ensure validity of the DI method.

The above authors presented elastic rebound behaviour of WC particles from various targets and found increasing coefficients of restitution and decreasing impact areas with increasing target hardness in a further communication [210]. Later, they extended their investigations to plastic deformation assessment of target materials and found varying crater characteristics comparing static to dynamic indentation [185].

WALL et al. [203] investigated the rebound behaviour of very small ammonium fluoride particles impinging upon a range of target materials with various velocities and particle sizes to obtain data for particle capture and energy dissipation. They introduced an energy-based impact formulation and found the coefficient of restitution to be dependent on particle diameter. This dependence was reported to be a function of impact velocity. Furthermore, they reported measurable differences in particle restitution coefficients depending on the target material and these differences were reported to be measurable only over a certain velocity range.

GONDRET et al. [63, 64] gave an overview of single-particle restitution behaviour for various particles rebounding from various target materials in a range of fluids without indentation or erosion. They reported the fluid playing a non-negligible role in the determination of coefficients of restitution. The normalized coefficient of restitution is reported to be a function of the near
3.5 Findings most important to this work

DRY-ICE INJECTION SYSTEMS

The only publication dealing with an Euler-Lagrange simulation of a dry-ice blasting nozzle known to date is from DONG et al. [48], who used Ansys CFX for a parameter study of the nozzle geometry. However, the particle tracking results were not validated against experimental results. Further numerical studies such as these by POUGATCH et al. [152, 153] and ADAMOPOULOS and PETROPAKIS [2] were focussed on particle tracking in flow regimes with high Mach numbers but these did not consider dry-ice particles.

To provide validation data for dry-ice blasting nozzle simulations, HSC experiments are presented in this work comparable those reported by UHLMANN et al. [198], REDEKER et al. [156, 157], SPUR et al. [176] and HABERLAND [72] from which the results by REDEKER et al. [156, 157] are the most detailed. Based on these findings a new HSC experiment is designed and particle properties of dry-ice blasting jets are measured in the corresponding recordings. Various nozzle types, operational modes and particle materials are considered. Special attention is paid to the post-processing methods used because these may be prone to complications triggered by the complexity of dry-ice jets such as reported by STRATFORD [180] or by LONGMIRE and EATON [111].

Numerical simulations of these above cases are carried out using a state of the art set-up utilizing 2-way coupling and neglecting modifications to the turbulence equations. Regarding this simulation set-up, general information about particle tracking can be found, for example, in the overview by GOUESBET and BERLEMONT [65] and more detailed in EPPLE et al. [53]. Possible coupling methods of the particles and the continuous phase were extensively discussed in
the latter publication as well as by LAIN and SOMMERFELD [106] and by HILTUNEN et al. [85]. Lain and Sommerfeld paid special attention to turbulence modifications by the particle phase, which, however, remain unconsidered in this work.

The numerical predictions of the particle tracks are compared extensively to the new experimental data for all nozzles and operational modes considered. Based on the results achieved for high Mach number flows a new empirical correlation for the drag coefficient is presented and, with this, the particle tracking predictions for these flows are improved. All the predictions above can be used to estimate boundary conditions for later engine defouling simulations.

PARTICLE BREAKUP MODELLING

The most extensive studies on dry-ice impact investigations are these by HABERLAND [72], REDEKER [156] and KRIEG [103]. These authors presented energy balances of the impacting dry-ice particles and paid special attention to potential phase change phenomena such as sublimation or, in the case of HABERLAND [72], melting upon impact. REDEKER [156] reported the particle breakup behaviour of dry-ice to be mainly dependent on impact velocity and particle diameter, which is confirmed with the experimental data presented here. All the above authors reported material properties of dry-ice in their studies. The basic energy balancing of the impact process as well as the material properties are adopted in this work.

This work presents an experiment for the investigation of single dry-ice particle impacts and the set-up is mainly influenced by what was reported in VARGAS et al. [200], HAUK et al. [77, 78], PAN and RENDER [143, 158] and GUEGAN et al. [69, 70] in their water-ice impact studies. Two high-speed cameras (HSCs) are used in this work to record single dry-ice particles impacting a variable target plate. The particles are accelerated by means of a gas-gun and particle sizing and tracking techniques are adapted from all the studies above.

The phenomenon of a densely-laden and fast dust particle cloud, which appears directly after the primary particle impact and which is reported in [69, 70, 77, 143, 158], is also observed for dry-ice. The secondary particle velocities of
dry-ice are assumed to be described by an elliptical envelope, similar to the behaviour observed by PAN and RENDER [143, 158] and GUEGAN et al. [69, 70] for water-ice particles. The general model assumption of ice fragmentation and the onset of breakup presented by HAUK et al. [77, 78] is also adopted for dry-ice in this study.

Furthermore, the main model assumptions of dry-ice fragmentation reported in this work are influenced by the granular particle based studies from RUSSELL [162] and ANTONYUK et al. [10, 11, 12], who experimentally and numerically investigated the breakup process of various materials. The authors also discussed potential correlations of the breakup process from impact variables.

All studies related to the research group of THRONTON et al. [96, 125, 181, 192, 193] are of high interest for the description of the dry-ice breakup process addressed in this work, since they deal with detailed DEM modelling of granulates and they provide an detailed insight into the breakup process in general. The fragmentation modes presented in the above studies were found to be dependent on diameter and either velocity or internal bond energy. The onset of breakup was discussed as a function of the modified Weber number, Eqn. (3.7), in these studies and a mass-based particle classification procedure was proposed.

The findings reported in [72, 103, 156] dealing with dry-ice particle impacts are taken into account for preliminary impact investigations. These investigations revealed that, taking into account the range of particle sizes and impact velocities considered in this work, the dry-ice particles disintegrate into significant numbers of secondary particles and that the proportions of sublimated mass are negligible. The 2D impact behaviour of water ice particles reported in [69, 143, 158, 200] was confirmed for dry-ice and, based on this finding, a new breakup experiment was designed to underpin a novel breakup model for dry-ice particles. The design of this experiment is comparable to what was reported in [143, 158, 200].

Two HSCs are used to record single particle impacts and to measure secondary particle features. A post-processing strategy comparable to what was described in [78, 200] is used for secondary particle numbers and sizes. Furthermore,
the strategy for tracking of secondary particles in a cloud is adopted from [143, 158]. The energy balances underpinning the dry-ice particle breakup process reported in [72, 103, 156] are enlarged in this work and subjected to a sensitivity analysis based on the application case. The resulting mass- and energy-balances are solved in the new breakup model utilizing the new experimental database. The mass based classification of secondary particles is adopted from [96, 125, 181, 192, 193].

These extensive experiments presented here permit a deeper insight into dry-ice impact and breakup behaviour. The new database is used to numerically predict dry-ice particle impacts in Euler-Lagrange simulations and this procedure is utilized in the later validation and aircraft engine defouling simulations.

**DEFOULING EROSION MODELLING**

The new erosion model presented in this work is based on an energy balance comparable to Eqn. (3.11) which is underpinned with data acquired by means of a single particle experiment comparable to the “Dynamic Indentation Testing” (DI) presented by HUTCHINGS et al [91, 92] and SUNDARARAJAN et al. [184, 194]. By means of this experiment, it is possible to determine the amount of energy necessary to penetrate and remove certain portions of typical foulants from aircraft compressor airfoils and to predict the amount of these portions removed.

The experiment is designed under consideration of the main conditions for DI testing reported in [184, 194]:

- quasi-static impact behaviour
- negligible stress-wave energy losses
- negligible particle rotation
- particle hardness must be greater than target (i.e. fouling) hardness
- superposition of erosion from normal and tangential forces is possible.

Following [91, 92, 101, 148] it is assumed that the defouling process is independent from the particle material and therefore reference material particles,
which do not disintegrate on impact, are used for rebound testing in this work. The results are scaled by means of empirical defouling functions to dry-ice particles. A procedure comparable to this was reported and extensively examined by Papini and Spelt in their decoating studies [145, 147, 148].

GONDRET et al. [63, 64] investigated various material pairings and reported similarity in their restitution behaviour if the coefficient of restitution is described as a function of the near-wall Stokes number, Eqn. (3.10). A similar procedure is used in this work to measure foulant properties with non-disintegrating particles made from reference material and to adapt these findings to dry-ice particles. Comparable normalization approaches have been reported in [18, 42].

Based on the findings reported in [18, 42, 145, 203] it is expected that the energetic properties of the defouling process are measurable only in a certain range of normal impact velocities. Furthermore, the angular dependence of the defouling rates is assumed to be dependent on the fouling material following [45], and brittle and ductile material behaviour is taken into account when the impact angles are declared for the new experiment (i.e. 90° and 30° measured parallel to the wall), following for example [37, 108].

The particle impact and rebound characteristics and the areas defouled are recorded with a HSC and a digital camera. An extensive database is recorded and the post-processed data reveals proportions of defouling energy for the whole range of impact velocities and diameters considered. Based on this data, logarithmic defouling functions are correlated for all particle and fouling materials considered and for both impact angles mentioned above. These functions underpin the new defouling erosion model for dry-ice particles and this is used to predict airfoil defouling in the later validation and application case studies.
4 Dry-ice injection system modelling

In this Chapter, experimental and numerical investigations of CO$_2$ dry-ice blasting nozzles are presented. The dependence of particle outlet velocities on system parameters and particle size distributions from various nozzle types are considered. Comparability of dry-ice blasting flows to flows laden with single POM particles is discussed. The main goal is to find an appropriate Euler-Lagrange formulation to make future parameter studies independent of expensive experiments and numerically efficient. A compromise solution between highly accurate numerical predictions and effective engineering has to be found which can work within tolerable uncertainties in the application case of commercial aircraft compressor cleaning simulations.

Section 4.1 contains the experimental validation study with a re-engineered transparent convergent-divergent dry-ice blasting nozzle and a POM particle laden flow. The geometry investigated and the experimental set-up of the HSC based PTV experiment are explained and the post-processing strategy is outlined. The main results, comprising particle tracks of various particle sizes and system pressure settings, are presented and discussed.

In section 4.2, the experimental outcomes from section 4.1 are used to validate an Euler-Lagrange particle tracking simulation using Ansys CFX. The numerical set-up and a validation study of pure air flows (using experimental data published elsewhere) is presented. Using this validated set-up, the above POM particle laden flow is simulated and compared to experimental data from section 4.1. An adequate set-up is found for all cases considered. However, it is detected that numerical particle tracks become significantly underpredicted when the nozzle pressure is increased in compressible flows.
Section 4.3 contains the experimental parameter study of three dry-ice blasting nozzles considered for axial compressor defouling experiments. These nozzles are operated in supersonic compressible, transonic compressible (here called sonic) and subsonic incompressible flow regimes. The experimental set-up is described, followed by a brief description and discussion of the post-processing strategy used to count, size and track the POM and dry-ice particles emerging from the nozzles. With the post-processed data, the blasting nozzles are characterized using cumulative probability functions which consider dry-ice particle sizes and velocities. Particle velocity differences are detected between dilute- and densely-laden dry-ice flows for all systems investigated. Good agreement is found between single POM particle tracks and tracks of large dry-ice particles from dilute-laden flows.

In section 4.4 all experimentally investigated dry-ice blasting nozzles are simulated using Ansys CFX and the Euler-Lagrange set-up from section 4.2. A pre-processing study is carried out to adjust the number of model particles and the air flow temperature to be considered. The main simulation outcomes are compared and discussed for various degrees of particle loading. Simulated results are then compared to the experimental results presented in section 4.3, where possible. This comparison shows that the numerical particle tracking set-up chosen is applicable for both incompressible and compressible flow regimes at low pressure settings. However, for the supersonic nozzle at high system pressure it fails to precisely predict POM and dry-ice particle tracks.

For the above reason, an additional study is presented in section 4.5 to improve the particle tracking predictions for supersonic nozzles. Based on an additional literature and theory review presented in section 4.5 the problem is analyzed theoretically and its physical complexity is highlighted. A re-engineering of experimental particle acceleration data from section 4.1 is presented and a new empirical drag coefficient correlation is derived from this data. This new correlation is implemented into Ansys CFX and new results from repeated supersonic nozzle simulations show the improvement desired. However, future work is required to generalize and physically underpin the new correlation presented.
4.1 Experimental validation study

This part of the study was mainly presented in: RUDEK et al. [1]

An experiment utilizing a high speed camera (HSC) in a multi-frame single-exposure setting is presented, which provides validation data for macroscopic particle transport simulations in a convergent divergent nozzle. Solid spherical particles made from POM with diameters from 1.5 to 3.0 mm are photographed passing through the transparent test nozzle. The particles are transported by compressed air at 2, 4 and 6 bar nozzle gauge pressure. An intensity based image post-processor is used to generate particle velocity information along the nozzle. The particle tracks are correlated and discussed with respect to possible uncertainties.

4.1.1 Set-up

The experimental set-up, shown schematically in Fig. 4.1, consists of the compressor (1) and the dry ice blasting machine (2). Single POM particles (3) are introduced into the compressed air flow by a slowly turning perforated disc system. The system pressure is preselected at (2). There is a 5 m long flexible connecting tube (4) linking the blasting machine with the transparent test nozzle set-up (5). Pressure losses in section (4) were estimated a priori and accounted for in the pressure setting. Pressure loss estimations indicated a range from 10 to 15 %, which is comparable to what was reported by REDEKER [156] for conventional dry-ice blasting nozzles. All given pressure values in this section are referred to as nozzle gauge pressure. The particles (3), which are introduced at position (2), are carried through (4) to the transparent testing nozzle (5). Here, the HSC (7) (PCO dimax4s, monochrome) is positioned parallel to the test section and the lighting system (6) (IES4412, 2 x 48.000 lm LED, 45° reflection beam) is arranged around it. The nozzle assembly is positioned 40 cm above ground.
A detailed view of the nozzle assembly investigated is given in Fig. 4.2. It displays the convergent divergent round Laval nozzle (region {0} to {R}) with key dimensions (all in mm). The throat is located at position {S}. This section of the nozzle is followed by a non-circular divergent part (region {R} to {L}). Its outlet square shape is rectangular (position {L}). The nozzle is made from transparent acrylic material by means of a high precision milling machine and subsequent stress relief heat treatment which ensures optical access into the nozzle. Its dimensions are re-engineered from an actual dry-ice blasting nozzle. The HSC equipment is positioned parallel to the vertical side of the outlet rectangle (not obviously clear from Fig. 4.1). Particle velocities measured are assumed to be approximately 2D, composed of axial and vertical components.
The HSC settings were adjusted depending on critical experimental variables. These are the maximum expected particle velocity (in this case 150 m/s) and the smallest particle diameter considered (in this case 1.5 mm) as well as the requirement of recording the entire nozzle in the field of view of the HSC. The maximum recording time of a single sequence was limited to 45 sec by cooling requirements of the high performance LED lighting system. The experimental restrictions resulted in a spatial discretization of 1875x290 pixel (px) and temporal discretization of 9,200 frames per second (fps) in conjunction with a nominal shutter speed of 1.28 µs. For each parameter set, 40 single particle tracks were recorded. This gives a total of 480 single particles being surveyed in the framework of this study, encompassing four particle diameters in conjunction with three pressure settings.

4.1.2 Results

The experiment described in section 4.1.1 is post-processed using background separation and a threshold valuing procedure. The particle positions are tracked utilizing the centre of mass (here the centre of intensity) based centroid matching approach. The related post-processing is described in more detail in section A.1 in the Appendix.

The particle tracks are correlated by means of a logarithmic equation

\[
\left| v_{P}^{[s]} \left( \frac{x}{L} \right) \right| = C_2^{[s]} \cdot \ln \left( \frac{x}{L} \right) + C_1^{[s]} \cdot (1 \pm K_{err}^{[s]}) \]  (4.1)

where \( C_i \) are curve fitting constants. These are derived by applying the least squares method to the experimental results, briefly described in section 5.3.2 and can be found in more detail in [26]. The indices 1 and 2 in Eqn. (4.1) refer to the order of the constants. The superscript \([s]\) stands for the relevant experimental parameters (i.e. system pressure and particle diameter pairing).

The variable \( K_{err} \) in Eqn. (4.1) represents an error estimate for each particular correlation. It comprises measurement uncertainties as well as the experimental scattering encountered. Table A.1 in section A.2 in the Appendix contains all relevant values of the corresponding constants from Eqn. (4.1).
Figure 4.3.: Experimental data-points and correlations from Eqn. (4.1); the blank gap at approximately $x/L=0.25$ relative nozzle length results from a poor SNR value in this region caused by a threaded connection.

Two reduced samples of experimental data points are shown in Fig. 4.3, incorporating the associated correlations from Eqn. (4.1). The left-hand image shows the dataset for 3.0 mm particles being accelerated at all nozzle pressure values considered. In the 2 bar set-up, the particles are not further accelerated because the flow starts to expand in the divergent nozzle section. This is the case at approximately $x/L=0.6$. To achieve a valid correlation for all cases based on a logarithmic function, the 2 bar cases are considered and correlated only until this position. In the right-hand image of Fig. 4.3 particle tracks of all investigated particle sizes and 6 bar nozzle pressure can be seen. A slight dependence of the particle acceleration on their size can be detected.

<table>
<thead>
<tr>
<th>Diameter</th>
<th>$K_{err}$ - 100 [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2 bar)</td>
<td>4 bar</td>
</tr>
<tr>
<td>1.5 mm</td>
<td>14 %</td>
</tr>
<tr>
<td>2.0 mm</td>
<td>15 %</td>
</tr>
<tr>
<td>2.5 mm</td>
<td>16 %</td>
</tr>
<tr>
<td>3.0 mm</td>
<td>17 %</td>
</tr>
</tbody>
</table>

Table 4.1.: Error estimate $K_{err}$ for the correlation from Eqn. (4.1) (note: 2 bar case valid until $x/L=0.6$ relative nozzle length).
Comparison of the trends displayed in Fig. 4.3 with corresponding values of the error estimate $K_{err}$ in Tab. 4.1 reveals the range of experimental scattering (i.e. lower scattering equals lower error estimate). For 3.0 mm particles it decreases, for example, from 17 % at 2 bar to 9 % at 6 bar. This trend is also observed for the other cases. Sporadic strong deviations of single particle tracks from the mean particle cluster were found during post-processing. Investigation of this phenomenon revealed individual particles encountering multiple wall collisions in the throat region of the nozzle causing the experimental scattering. However, some particles were found to be trapped in the throat region for several time steps. The trapped particles were determined to be unrepresentative and removed from the evaluation.

**Figure 4.4.:** HSC recordings of a single POM particle in the transparent nozzle from Fig. (4.2), typical SNR values above.

The blank gap at approximately $x/L=0.25$ relative nozzle length in Fig. 4.3 results from a poor SNR value in this region. The threaded connection between round and rectangular nozzle is not optically accessible so there is no experimental velocity information available. Figure 4.4 contains some consecutive, instantaneous recordings of a single POM particle inside the nozzle. The threaded connection can be seen and it is indicated by typical SNR values at the top of Fig. 4.4.
4.2 Numerical validation study

This part of the study was mainly presented in: RUDEK et al. [I]

The validation of a possible numerical set-up is carried out considering the above given case simulating the single POM particles. Based on preliminary geometry and grid studies (not reported here), the simulation strategy is tested for pure air flows against experimental data from literature [79, 144]. Particle laden flows are then validated against experimental data presented in the above section 4.1.2. Some possible simulation set-ups are discussed and the best case is selected for later parameter studies with dry-ice.

4.2.1 Set-up

The simulations presented here are conducted using the commercial software Ansys CFX 15.0 and 16.2. No modifications of the software have been made. The continuous phase, here compressed air, is simulated considering mass, momentum and energy conservation equations. Compressible flow is assumed and therefore the total energy approach is chosen for the simulations. It includes viscous heating and variable density effects. To account for turbulent fluctuations, the RANS $k - \varepsilon$ turbulence model is chosen. The turbulence model constants are maintained at standard values and dispersed phase induced turbulence modification is not considered, because there is no such opportunity in the standard CFX toolbox. To achieve final closure of the system of conservation equations, air is modelled as ideal gas, relating density to pressure and temperature as well as specific heat to temperature.

The boundaries of the CFD model representing the experimental set-up are assumed to be adiabatic. There is no heat-transfer considered between the phases. However, to account for possible heat-transfer between dry-ice particles and fluid in the linking tube in later simulations (see Fig. 4.1 - pos. (4)), an a priori temperature estimation was performed, which is described in section 4.4.1. By means of this, fluid temperature at the nozzle inlet can be adjusted in case of densely laden dry-ice flows. This is not necessary for simulations with POM
particles or dilute laden dry-ice flows. As can be seen from Fig. 4.5, the nozzle and an appropriate portion of ambient volume are simulated using a 90° symmetry 3D model. Gravity is therefore neglected in the simulations of the supersonic and the later sonic nozzle. A 180° section is selected if gravity must be considered (later with the subsonic nozzle). Additional details about the numerical set-up are presented in section A.3 in the Appendix and Tab. A.2 summarizes all relevant information.

Furthermore, representative comparison data between air flow simulations and experimental data from literature [79, 144] as well as results from 2D simulations presented by HELL et al. [79] are considered for validation of the above set-up. These studies deal with compressible subsonic and supersonic flows in two slightly different, axisymmetric, convergent divergent nozzle geometries. All measurements were conducted by conventional pressure probe and by Laser Induced Thermal Acoustics (LITA) [58, 79, 80]. The corresponding nozzle geometries were generously supplied by the authors of the relevant publications [58, 79, 80]. All important operating conditions can be found in the aforementioned publications. The subsonic test case chosen is from PANCHAPAKESAN and LUMLEY [144]. It was designed to investigate an undisturbed subsonic free jet towards higher order moments for assessment of Reynolds stresses. All relevant measurement was conducted by thermal anemometry. The nozzle geometry and the corresponding boundary conditions are taken from [144].
Figure 4.6.: Compressible subsonic test case - relative static pressure along nozzle wall; num. results vs. num. and exp. data from [79].

Figure 4.6 contains a typical result from the validation study. The comparison of static wall pressure ratio in the subsonic case is plotted over relative nozzle length and the corresponding test-nozzle is shown. The throat of the nozzle and the beginning of the constant cross section are marked in the figure. Experimental and numerical data from [79] is compared to results of the validation simulation from this study. A normal shock develops at the nozzle exit (i.e. relative nozzle length x/L=1) and it adjusts static to ambient pressure [79].

The pressure fluctuations upstream this shock can be attributed to a shock system which develops because the nozzle is operated in a non-matched operational mode [79]. The predicted pressure field results at the wall can be seen to be in good agreement with the corresponding experimental and numerical results from [79]. In the region of the shocks (starting at relative nozzle length of approximately x/L=0.5) the simulations tend to underpredict the experimental results.

The number of shocks (i.e. four) occurring in the nozzle is the same for experiment and simulations. The position of the third shock is simulated to be further downstream compared to the corresponding experimental indication. The simulation data from [79] and the simulation results presented here approximately coincide. The same conclusions can be drawn for the Mach number profiles and velocity profiles compared and this is discussed in detail in section A.3 in the Appendix. The mean deviations for all data compared are found to range from 3 % to 13 %.
4.2.2 Results

To validate the particle tracking procedure, unladen air flows of the validation nozzle (Fig. 4.2) were simulated with the set-up documented in section 4.2.1. Three system settings (i.e. nozzle gauge pressures of 2, 4 and 6 bar) were considered, corresponding to the validation experiments presented in section 4.1. Figure 4.7 shows the bulk flow Mach number development along the normalized nozzle axis (x/L) and provides an insight into the flow states which were chosen for the validation experiment.

![Mach number along nozzle/jet axis from pure air flow simulations (left); Mach number contour at 4 bar showing separation phenomena (right).](image)

The 2 bar setting results show that the flow at the outlet of the nozzle (relative nozzle length = 1) is subsonic and that an expansion starts already in the nozzle at a relative nozzle length of approximately x/L = 0.6. In case of 4 bar nozzle pressure, outlet Mach number oscillates and the flow state is referred to as transonic. In the last case, nozzle pressure of 6 bar, the outlet Mach number has a value of approximately 2 and the flow is expanded in the emerging jet. This situation is referred to as supersonic in what follows.

The Mach number oscillations inside the nozzle (i.e. at 2 bar and 4 bar) can be attributed to asymmetric boundary layer and shock separations which are caused by the non-matched operational mode of the nozzle. Such a situation is shown in the right-hand side of Fig. 4.7 for the 4 bar setting as a result from
the simulations. A restricted shock separation with downstream reattachment develops at the short nozzle wall (i.e. z-direction) and a free shock separation develops at the long nozzle wall (i.e. y-direction). These separations form a complicated system of shocks and expansion waves, which is additionally influenced by the rectangular shape of the nozzle, and this system significantly influences the main flow which is represented by the Mach number trends discussed in Fig. 4.7. The flow behaves comparable to an overexpanded jet, in which Mach number fluctuations are triggered by the interaction between the free shear layer and the shock and wave pattern. Details about the separation phenomena encountered here and possible corresponding Mach number fluctuations can be found for example in [49, 73, 124, 178].

Furthermore, the coupling methodology as well as the forces contributing to the ODE of motion of the particles, Eqn. (2.64) and (2.73), were parametrized in the study and this is presented in detail in section A.4 in the Appendix. The 2-way coupled formulation including drag and pressure-gradient forces is determined to be the best set-up option tested and the mean deviations encountered are in the range from 5 % to 10 % and vary slightly. Comparing the deviations discussed here to those encountered during the air flow validation study, which is documented in section 4.2.1, reveals them to be of the same order. An evaluation of the magnitude of the deviations of numerical values from experimental values in relation to experimental variance shows that the mean numerical predictions fit the experiment well with respect to its maximum scattering. This is shown in Fig. 4.8 for two typical examples.

The results simulated are compared to the mean experimental trends presented in section 4.1.2 and to the experimental scattering boundaries. These scattering boundaries are plotted as dash-dotted trend lines in Fig. 4.8 above and below the mean experimental trends and they are derived from the slowest and the fastest particles encountered in the experiments. The left-hand side of Fig. 4.8 compares the trends for the smallest 1.5 mm POM particles and 4 bar system pressure. The right-hand side shows the same situation for the largest 3.0 mm POM particles and 6 bar system pressure.
**Abbildung 4.8.**: Typical results from scattering study: 1.5 mm POM particle tracks at 4 bar, (left) and 3.0 mm POM particle tracks at 6 bar (right); comparison of trend lines from simulation and experiment with experimental scattering indication.

The mean tracks predicted are close to the mean experimental values in the 4 bar case but these predictions for 6 bar are close to the lower scattering boundary of the experiment. All predictions are found to be inside the experimental scattering boundaries in the cases considered even if the mean experimental trends are clearly underpredicted, such as in the 6 bar case presented above. The whole scattering study is discussed more detailed in section A.4 in the Appendix.

Figure 4.9 shows the final numerical results from 2-way coupled simulations with drag and pressure-gradient force consideration for particle tracks compared to corresponding experimental trends. The upper left diagram shows data for the smallest particles investigated, 1.5 mm, conveyed at three nozzle pressure settings. The upper right diagram contains the same set of information for 2.0 mm particles and the lower diagrams contain trends for 2.5 mm particles (left) and 3.0 mm particles (right). In general, the trends for all particle sizes appear to be comparable.

Numerical data can be seen to be in good agreement with experimental data in case of the lowest pressure setting, underpredicting the experimental outcomes at a nozzle pressure of 4 bar and more significantly underpredicting the experiment at 6 bar nozzle pressure. These tendencies indicate that the numer-
4.3 Experimental parameter study

This part of the study was mainly presented in: RUDEK et al. [II]

An experiment with a HSC is presented to investigate the behaviour of dry-ice particles at the outlet of various dry-ice blasting nozzles. Measurements are made using a range of representative blasting systems in typical configurations.
with various dry-ice particle mass fluxes. Particle size distributions and particle velocity distributions are compared for the investigated range of systems and parameters. A comparison between dry-ice particle laden flows and flows with single POM particles in the above given range of diameters (see section 4.1) is discussed.

4.3.1 Set-up

The experimental set-up for the nozzle investigations presented here varies only slightly from what is described detailed in section 4.1.1 for the initial validation study with POM particles. The schematic from Fig. 4.1 is shown in a modified version in Fig. 4.10. The principle of operation is described in section 4.1.1.

All given pressure values in this section are referred to as system pressure, which is preselected at (2). The HSC (7) (PCO dimax s4, monochrome) is positioned parallel to the particle laden free jet emerging from the nozzle (5) and the lighting system (6) (IES4412, 2 x 48,000 lm LED, 22,5° reflection beam) is arranged around it. The background behind the free jet is painted black to achieve a strong contrast to the particles. The nozzle assembly is positioned 40 cm above ground. The investigated area of the free jet begins directly after the nozzle outlet and comprises 50x35 mm, which is emphasized schematically in Fig. 4.10 (yellow area).

The first two nozzles used are the standard convergent divergent blasting nozzle from the above validation study (sections 4.1 and 4.2), providing a supersonic outlet air flow with system pressure of 8 bar (referred to as su-

![Figure 4.10.: Schematic of the experimental set-up.](image-url)
personic nozzle #1) and a convergent nozzle, providing a sonic outlet air flow while operating at system pressure of 2 bar (referred to as sonic nozzle #2). Both nozzles have a rectangular (flat) shaped outlet area and their inlets (link between (4) and (5) in Fig. 4.10) are circular.

![Diagram of nozzles](image)

**Figure 4.11.** Detailed 3D section view of nozzles investigated, sonic nozzle #2 (left) and subsonic nozzle #3 (right).

The third nozzle investigated is a subsonic particle accelerator (referred to as subsonic nozzle #3) which is driven by an air-blower. Dry-ice particles are introduced directly into the air flow from a container placed above the flow channel. Figure 4.11 shows detailed views of nozzles #2 and #3. Details of nozzle #1 can be seen in Fig. 4.2 (section 4.1).

The outlet flow pattern of the particles is investigated in 2D and the component of the velocity vectors in the depth direction is assumed to be negligible. The HSC is operated with spatial discretization in the range from 16 to 44 px/mm and temporal discretization in the range from 10,000 to 35,000 fps. The shutter speed is set to 1.28 $\mu$s. These settings theoretically permit the sizing of particles as small as 45 $\mu$m (with 44 px/mm, assuming that an instance of particle detection must consist of at least three pixels) and to track particles at maximum velocities up to 1400 m/s (with 35,000 fps, assuming a maximal displacement of 80 % of the axial length of the field of view of the HSC and that a particle must be detectable at least twice in this field of view).
The tracking algorithm utilized theoretically allows the matching of blurred particles. The whole post-processing procedure is described in detail section A.5 in the Appendix and it is briefly summarized in the following.

The HSC recordings are filtered in frequency domain and noise is reduced by application of selective and bandpass filtering functions. Background and particle information is distinguished by means of the clustering method presented by OTSU [142]. If this method fails to cluster the intensities of the frame appropriately a modified estimator proposed by YANG et al. [208] is used. If this method also fails, the frame is removed from post-processing.

A run-up study shows that the exact size information content of the image is varied by the above procedure, but the general trend of the particle size distribution is still captured (for details see section A.5 in the Appendix). An assessment experiment with POM particles of various sizes (i.e. particle diameters from 0.5 mm to 3.0 mm were considered) and shapes (i.e. spherical particles and non-spherical granules were considered) revealed a predictive accuracy of +/-6.5 % in particle diameter for the method which is assumed to be the maximum deviation encountered with the above procedure.

The ambiguity problem of automatized particle association for particle tracking in these dry-ice flows is solved by utilizing an idea originally presented by HERING et al. [82], who reported that a unique matching criterion for particle laden flows with up to 800 particles per frame-pair can be found if the particle size and its pixel energy (i.e. the grey value continuity) is taken into account resulting in the modified streak-overlapping technique (details can be found in section A.5 in the Appendix).

The physical plausibility of all possible particle matches is checked by means of a criterion to quantify the agreement of matched particle shapes in both frames. The direction of motion of the particles serves as a second plausibility criterion, allowing only a maximum limit for valid matches based on a priori estimated limits.

The 2D velocity vectors of the remaining particle pairs can be estimated automatically using centroid matching. A comparison study in which automatically generated particle tracks from the procedure presented above and in more de-
In summary, the PTV based post-processor used in what follows can size and track particles in particle laden flows with up to 800 particles per frame considering the following limitations and accuracy:

- user defined sizing aspect ratio limit for Eqn. (A.12): i.e. $AR_{\text{MAX}} = 0.25$
- user defined particle pairing criterion limit for Eqn. (A.17): i.e. $C_{i}^{\text{MAX}} = 0.90$
- user defined particle pairing shape limit for Eqn. (A.18): i.e. $C_{\text{ecc}}^{\text{MAX}} = 0.75$
- a priori estimated maximum flow angle limit for Eqn. (A.20): i.e. $\gamma_{\text{MAX}} = 5^\circ$
- common particle tracking matches per frame pair: 3 - 5
- sizing accuracy (equivalent diameter): +/-6.5 %
- tracking accuracy (absolute velocity): +/-5.0 %

4.3.2 Results

Particle laden flows from three different nozzle geometries introduced in section 4.3.1 are investigated with the experimental set-up and post-processing strategy presented above. The convergent divergent supersonic nozzle #1 (Fig. 4.2) is operated at 8 bar system pressure, the convergent sonic nozzle #2 is operated at 2 bar and the subsonic injection system (nozzle #3) is operated at 100% electrical power of the blower (P100) (both displayed in Fig. 4.11).
Three particle loadings of the flows are considered:

- single POM particles (single particle laden)

- low CO$_2$ dry-ice mass fluxes (dilute laden, 5%) - $\theta (m_{\text{CO}_2}) \sim 1\, \text{kg/s}$

- high CO$_2$ dry-ice mass fluxes (fully laden, 100%) - $\theta (m_{\text{CO}_2}) \sim 100\, \text{kg/s}$

Particle flow behaviour from all nozzles was first investigated with single POM particles. Ideal spherical POM particles with diameters from 1.5 to 3.0 mm were injected into the flow and blasted at all above system configurations. At least 40 POM particles were recorded and tracked downstream the nozzle outlets. Main outcomes from this experiment are shown in Fig. 4.12 and compared to data from dilutely laden dry-ice flows.

![Figure 4.12](image-url)

**Figure 4.12.:** Mean velocity trends of large dry-ice particles and single POM particles from blasting nozzles #1, #2 and #3.

Detailed investigations into these dilutely laden flows revealed the necessity to distinguish between large ($d_p \geq 1\, \text{mm} \rightarrow L$) and small ($d_p < 1\, \text{mm} \rightarrow S$) dry-ice particles. Velocities of large particles can be correlated as a function of their size for constant system pressure whereas this is not possible to a satisfactory degree for small particles. Tracks of large dry-ice particles are comparable to these of POM particles of comparable sizes.

For subsonic nozzle #3 POM velocities are found to be slightly higher compared to dry-ice velocities. In general there is no significant difference between
single particle POM flows and dilute laden dry-ice flows. Possible thermal ef-
fents due to heat-transfer from air to particles (i.e. cooling of air and consequent
changes of flow properties - see also section 4.4.1) appear to be negligible for
transportation of large particles in dilute laden dry-ice flow.

Figure 4.13 shows representative snapshots of dilute laden dry-ice flows from
all systems investigated. The leftmost image represents a flow situation found
to be typical for supersonic nozzle #1. A large particle can be seen, which is
surrounded by many small particles and dust. The centre image of Fig. 4.13
shows typical still for sonic nozzle #2. The flow pattern is dominated by mean
particle sizes, there are almost no large particles detected and there is less dust
contained compared to the flow pattern from nozzle #1.

The rightmost image shows a typical situation for subsonic nozzle #3. Mostly
large particles, even a number of unbroken original dry-ice pellets are visible.
Some smaller fragments can be seen in this flow pattern, too. The pressure-less
injection system (nozzle #3) delivers the largest dry-ice particles of the sys-
tems investigated and supersonic nozzle #1 delivers more large dry-ice particles
compared to sonic nozzle #2.

This qualitative finding is quantified with cumulative particle size distributions
shown in Fig. 4.14, left. To determine these trends, a number of samples from
HSC recordings were taken at random instants of time. Each trend shown in
Fig. 4.14, left, contains size information from at least 40,000 single dry-ice
particles. The cumulative trend for nozzle #1 reveals a wider spread in particle
sizes than this for nozzle #2. It shows a larger proportion of small particles but
also contains solitary larger particles compared to nozzle #2. Comparison of es-
Estimated mean diameters reveals a size of $d_p \approx 225 \mu m$ for both nozzles #1 and #2 but higher variance is encountered for nozzle #1. The cumulative trend for nozzle #3 is most widespread and the mean particle diameter of $d_p \approx 875 \mu m$ is significantly higher compared to both other nozzles. Particle size distributions were found to be independent of mass flux for all nozzles investigated.

![Graph showing particle size and velocity distributions](image)

**Figure 4.14.** Particle size distributions (left) and particle velocity distributions (right) in dry-ice flows from blasting nozzles #1, #2 and #3.

The right-hand graph of Fig. 4.14 shows the corresponding trends of dry-ice particle velocities. Here, global cumulative trends containing information from all particles detected are discussed for fully laden flows. Nozzle #1 delivers particles at highest velocities (mean value $v_p \approx 250 m/s$) and largest scattering of particle velocities compared to the other nozzles. Particle velocities from nozzle #2 are significantly lower (mean value $v_p \approx 75 m/s$) and less widespread and nozzle #3 delivers the slowest particles (mean value $v_p \approx 20 m/s$) with only a low velocity scattering.

A more detailed investigation of particle velocities dependent on various degrees of particle loading and on particle size (distinguishing large ($d_p = L$) and small particles ($d_p = S$) as proposed above) leads to the results discussed in Fig. 4.15 to 4.17.
Figure 4.15.: Particle velocity distributions for large (L) and small (S) particles in dry-ice flows from blasting nozzle #1 with 5% and 100% mass loading.

In Fig. 4.15, cumulative probability trends for supersonic nozzle #1 at dilute (5%) and dense laden flow state (100%) are compared. These trends are normalized by the maximum velocity detected with this nozzle. Large particles exit nozzle #1 at more homogeneous velocities compared to small particles at both mass-loading states. Scattering for both, large and small particles, is comparable for both mass-loadings. Increasing mass-flux increases mean large particle velocities by approximately 5% and small particle velocities by 10%. This effect can be explained with local and temporal flow modifications caused by large or multiple particles at certain instants of time inside the narrow sections of the nozzle (detailed discussing in section 4.5).

Trends for sonic nozzle #2 are discussed in Fig. 4.16. Particle velocities are normalized by the maximum velocity encountered for nozzle #2. The trends show significantly decreasing velocities of small particles at increased mass-loading compared to the dilute laden flow. Scattering of small particles velocities also decreases. The velocities of the large particles remain comparable for both mass-loadings but scattering of larger sized particles decreases with increased mass-load. Higher mass-loading seems to decelerate the continuous flow significantly and leads to lower overall particle velocities for nozzle #2.
Figure 4.16.: Particle velocity distributions for large (L) and small (S) particles in dry-ice flows from blasting nozzle #2 with 5% and 100% mass loading.

Experimental results for nozzle #3 are discussed in Fig. 4.17. It reveals another correlation of flow states and particle sizes compared to the nozzles above. All trends are again normalized by the maximum velocity encountered for this nozzle. Increased mass-loading aligns mean velocity values of small and large particles and increases the overall velocity scattering. The mean velocities of

Figure 4.17.: Particle velocity distributions for large (L) and small (S) particles in dry-ice flows from blasting nozzle #3 with 5% and 100% mass loading.
large particles are increased while these of small particles are decreased. For some particles, however, there are significantly larger velocities found in the dense flow compared to the dilute laden flow. This behaviour can be attributed to the unsteady and discontinuous loading when injecting a high number of particles into the flow of this system. The subsonic flow is significantly affected if large proportions of dry-ice are injected. Conversely it is more stable if only few particles are injected.

4.4 Numerical parameter study

This part of the study was supported by BERGHOFF, G. [III] and his work was supervised by the author.

This section describes final simulations of the above typical dry-ice blasting flows for commercial aircraft compressor defouling. The simulations presented comprise all cases discussed in section 4.3, namely supersonic nozzle #1 at 8 bar system pressure, sonic nozzle #2 operated at 2 bar system pressure and the blower driven subsonic nozzle #3. All particle loading states, single POM particles, dilute and dense laden dry-ice flows, which are described in section 4.3.2, are considered for the simulations presented here. Results are compared to experimental outcomes and final conclusions are drawn from this comparison.

4.4.1 Set-up

The nozzles used in the experiments and all flow states considered in section 4.3.2 were simulated numerically and the numerical set-up is based on the preliminary grid and set-up studies reported in section 4.2. Details of the numerical configuration are also reported in the aforementioned section. The numerical set-up is summarized in detail in Tab. A.2 in section A.3 in the Appendix.
Particle phase modelling

The important link between experimental particle size distributions, the number rate distribution in the simulation and the mass flux of the particles is described in detail in section A.6 in the Appendix. The most important dependencies are briefly explained below.

Experimental size distributions of dry-ice particles, \( p_{\text{exp}}(d_p) \), are modelled in six representative particle size classes \( c = 1...N \) (here \( N = 6 \)) in the simulations presented in this section

\[
d_p^{[c]} = [125...4000 \mu m] ... c = 1...6. \tag{4.2}
\]

Their probability densities can be derived directly from experimental data and this is described in more detail in section A.6 in the Appendix. The number-rate describes the number of real particles represented by a single Lagrangian model particle in the simulations per unit time. It is defined as follows:

\[
\dot{n}_c = \frac{\dot{m}_c}{m_c} \tag{4.3}
\]

where \( \dot{m}_c \) is the mass flux of a certain particle size class and \( m_c \) is the mass of a representative particle from this class. A link between the classified particle size distribution \( p\left(d_p^{[c]}\right) \) and the particle number-rate distribution \( p\left(\dot{n}_c\right) \) has to be formulated for each particle size class \( c \) (see section A.6, Appendix).

In all simulations presented in this section, the number distribution of numerical model particles \( p\left(n_p^{[c]}\right) \) is chosen to be uniform for all particle size classes \( N \) considered, i.e.:

\[
p\left(n_p^{[c]}\right) = \frac{1}{N} \tag{4.4}
\]

The simulation uses the known total particle mass flux \( \dot{m}_p \) and a chosen total number of model particles \( n_{p,\text{tot}} \). The latter influences the accuracy of the predictions and must be calibrated in a-priori set-up calculations, which was done...
in this study with nozzle #1 at 8 bar nozzle pressure. The main results from these initial calculations are discussed in section A.6 in the Appendix. Based on these results, the number of model particles $n_{P,\text{tot}}$ considered in what follows was selected to be 1,000 because it delivers almost the same results as the slightly more accurate solution with 10,000 model particles but it turned out to be much more efficient for the numerical solution process.

**Temperature effects**

Dry-ice particles are transported by compressed air via inking tubes from the blasting machines to nozzles #1 and #2 (see Fig. 4.10, pos. (3) to (5)). Heat transfer from the air to the particles is possible because there is a significant temperature difference between the compressed air (ambient temperatures of 15 to 20°C are maintained for the compressed air by a multiple-stage inter-cooled compression process) and the dry-ice particles (-78.5°C) at the injection region. As a consequence air temperature may decrease.

Air temperature affects the thermodynamic properties of compressed air (see Chapter 2) and hence the transportation and acceleration behaviour of particles in the flow. To account for this, an estimation of air temperature at the inlet into the nozzles (i.e. end of linking tube, pos. (4) in Fig. 4.10) must be considered. This is not necessary for nozzle #3, where particles are directly introduced into the nozzle air flow.

---

**Figure 4.18.** Schematic of the temperature estimation procedure.
To account for such heat transfer, a 1D model calculation has been set-up to estimate air inlet temperatures to the nozzles. This calculation procedure is illustrated schematically in Fig. 4.18 and it is described in more detail in section A.6 in the Appendix. Based on the results discussed in the aforementioned section, the approach from Fig. 4.18 is assumed to be a good estimation procedure for air temperature predictions of densely-laden dry-ice flows in nozzles #1 and #2. Results from final estimations for both nozzles are shown in Fig. 4.19. The air temperatures predicted at the end of the tube are considered as nozzle inlet air temperatures in the simulations discussed below. These are -77.8°C for nozzle #1 and -63.8°C for nozzle #2.

![Figure 4.19: Air temperature trends from 1D a priori estimation for fully-laden dry-ice flows in the linking tubes of nozzle #1 and nozzle #2.](image)

### 4.4.2 Results

In this section, the main representative results from numerical simulation of nozzles #1, #2 and #3 are discussed. All particle loading states introduced in section 4.3 are considered. Mach number contours are shown in Fig. 4.20 and these are plotted on a cut plane along the height axis of the simulated volume of nozzle #1. Only the most significant difference detected in the contours is displayed, which is that between unladen air flow (upper display) and fully-laden flow (lower display).
Figure 4.20.: Mach number contours of supersonic nozzle #1 at unladen (upper) and fully laden (lower) flow.

The influence of dry-ice particles is clearly visible, especially from lower Mach numbers along the nozzle “axis”. One should keep in mind that air temperature is decreased for fully laden flows. This is discussed in the above section 4.3.2. It leads to decreasing air velocities due to increased densities when maintaining a constant air mass flux.

Differences between various loading states become clearer when discussing Fig. 4.21. Here, Mach number trends for all particle loadings are plotted as a function of relative nozzle length along the “axis” of nozzle #1. Mach number decreases with increasing particle mass flux. Even the single POM particle flow influences the Mach number trend and this trend is comparable to the dilute laden dry-ice flow (5%). The most significant influence is clearly visible from full dry-ice loading (100%).

Mach number profiles along the height axis of nozzle #1 are discussed in Fig. 4.22. Two typical downstream positions (i.e. x/D = 1 - left-hand graph and x/D = 10 - right-hand graph) are presented. Only slight differences resulting from various low particle loadings can be detected compared to unladen air flow, but fully laden flow profiles clearly diverge from the others.

This fully laden free jet tends to widen at further downstream locations (Fig. 4.22 - right-hand graph compared to left-hand graph). A shock cell struc-
Figure 4.21.: Mach number trends for supersonic nozzle #1 with various particle loadings along the nozzle axis.

ture at outer radii of the jet locally accelerates the flow, which can also be seen from the contour plots above (Fig. 4.20).

Contours comparable to the above are shown in Fig. 4.23 for sonic nozzle #2. The most significant difference is encountered if comparing unladen air-flow (upper image) to fully laden dry-ice flow (lower image). The jet expands into a supersonic regime after passing the nozzle’s throat, which is also its outlet. The deceleration of the flow by particles is not as significant as detected for

Figure 4.22.: Mach number profiles (along height) for supersonic nozzle #1 and various particle loadings at downstream positions x/D = 1 (left) and x/D = 10 (right).
nozzle #1. There are only slight differences visible between the upper and the lower Mach number contour plots in Fig. 4.23.

This situation is confirmed by the trends displayed in Fig. 4.24, where Mach numbers are plotted along the nozzle “axis” as function of relative nozzle length x/L. A slight difference of the Mach number trend is visible only for the fully laden flow compared to all other trends with lower mass loadings.

Comparison of Mach number profiles for nozzle #2 is discussed in Fig. 4.25 at downstream positions x/D = 1 (left-hand side graph) and x/D = 10 (right-hand side graph) along the height coordinate of the jet. No significant difference between these profiles can be detected. Only the fully laden flow profile diverges slightly.

Mach number contours for subsonic nozzle #3 are compared in Fig. 4.26. This simulation was made considering 180° symmetry and buoyant forces in both the continuous and the particle phase. Therefore this nozzle is plotted in a total section view and only the interesting part of the lower ambience is considered. The most significant difference encountered for these Mach number contours can be found again comparing unladen air-flow (upper image) to fully laden dry-ice flow (lower image). Particle injection from the hopper above the nozzle

![Mach number contours for sonic nozzle #2 at unladen (upper) and fully laden (lower) flow state.](image)

**Figure 4.23.** Mach number contours for sonic nozzle #2 at unladen (upper) and fully laden (lower) flow state.
Figure 4.24.: Mach number trends for sonic nozzle #2 at various particle loadings.

influences the air flow mainly in the upper half of the nozzle, which can be clearly seen in the lower display of Fig. 4.26.

This influence of the upper half of the air flow is also detectable in Mach number profiles (here plotted along the whole radius of the jet), which are displayed in Fig. 4.27. Comparison between fully laden profile and all other trends at downstream position $x/D = 1$ (left-hand display of Fig. 4.27) clearly indicates particle’s influence upon the air flow.

Figure 4.25.: Mach number profiles (along height) for sonic nozzle #2 and various particle loadings at downstream positions $x/D = 1$ (left) and $x/D = 10$ (right).
Slight differences between dilute laden dry-ice flow and Mach number profiles from POM particle laden and unladen air-flow can also be seen in the upper half of the profile at \( x/D = 1 \). Further downstream, at \( x/D = 10 \) (right-hand side of Fig. 4.27), no such radial differences are detectable and only a slight difference between fully laden flow profiles these from the other particle loadings remains. The free jet becomes axisymmetric for all cases at this position.

**Figure 4.26.**: Mach number contours for subsonic nozzle #3 at unladen (upper) and fully laden (lower) flow state.

**Figure 4.27.**: Mach number profiles for subsonic nozzle #3 and various particle loadings at positions \( x/D = 1 \) (left) and \( x/D = 10 \) (right).
Finally, numerically predicted particle velocities at nozzle’s exit are discussed in the following Figures 4.28 and 4.29. POM particle flows (POM), dilutely-laden (5 %) and densely-laden (100 %) dry-ice flows are considered. These plots also contain experimental results (which are discussed in detail in section 4.3.2).

Results from POM particle investigations are discussed in Fig. 4.28. Good agreement is achieved between computational predictions for subsonic and sonic nozzle and experimental data. The computed supersonic particle velocities tend to underpredict by approximately 24 % compared to experimental results. This finding is in line with findings from the validation study, which is discussed in detail in section 4.2.2. Outlet particle velocity differences for the validation case at 6 bar were approximately 10 % and it was found that the underpredictive tendency of computations increases with increasing operating pressure of the supersonic nozzle.

In Fig. 4.29, left, computed particle velocities for dilute laden dry-ice flows are plotted as a function of particle size compared to experimental results in the possible ranges (see discussion in section 4.3.2). A good overall agreement between computations and experimental correlations can be seen for nozzles #2 and #3. Computational results of dry-ice flows from nozzle #3 slightly overpredict the experiment and these from nozzle #2 slightly underpredict the experimental trends.

![Figure 4.28.](image)

**Figure 4.28.:** POM particle velocities, comparison of computed and experimental results for all nozzles investigated.
Figure 4.29.: Dry-ice particle velocities, comparison of computed and experimental results for all nozzles investigated, dilutely-laden (left) and densely-laden flow (right).

Significant differences between calculated particle velocities from nozzle #1 and experimental results are also detected for dilute laden dry-ice flow. The mean underprediction is approximately 21% and corresponds to the above finding for POM laden flows. This underprediction becomes more significant (i.e. higher than 35%) for numerical predictions of fully-laden dry-ice flow, which is shown in Fig. 4.29, right.

The trends from both other nozzles #2 and #3 are in good agreement with the corresponding experimental results. Simulations of nozzle #3 slightly overpredict the experimental outcomes and those of nozzle #2 slightly underpredict the related experimental results, which is comparable to findings for dilute laden and single POM particle flows.

The outcomes from the parameter simulations presented here are acceptable for nozzles #2 and #3. However, significant underpredictions of experimental data are found for simulations of supersonic nozzle #1. This situation needs improvement and hence the numerical strategy is modified, which is addressed in the following section 4.5.
4.5 Improved estimate for drag coefficient in high-speed flows

To overcome the underpredictive nature of the numerical set-up in supersonic flow situations, an additional study intending a possible modification of the drag coefficient formulation in flows with high acceleration potential (i.e. high pressure flows) is presented. An additional literature survey towards possible formulations of drag coefficients in supersonic nozzles and a theoretical problem survey are presented in section 4.5.1. Based on these findings a re-engineering procedure of experimental drag coefficients is described and a new empirical formulation for the drag coefficient of POM and dry-ice particles in compressible flows is presented in section 4.5.2. All the above unsatisfactory simulations are repeated and a significant improvement of the particle velocity predictions is achieved.

4.5.1 Theoretical problem investigation

Numerous studies were found and examined dealing with particle acceleration in supersonic free flow conditions, however, none of those did reveal a valid formulation for the cases considered here (i.e. particles of non-negligible sizes in a convergent-divergent nozzle). The most important studies to this work are summarized below. Table 4.2 gives an initial overview of Mach and Reynolds number ranges as well as the investigative approaches of these studies.

BAILEY and HIATT [15, 16] reported experimental investigations in a wide range of Mach and Reynolds numbers on free flow drag coefficients of spheres. They found most significant changes to drag coefficients depending on Mach number in transonic range (i.e. $0.7 < Ma < 1.3$). Furthermore, the authors discussed possible contributors to drag coefficients and subdivided them to fore- and afterbody pressure. Forebody pressure was found to increase and afterbody pressure to decrease with increasing Mach numbers. In the later communication [16] the most important findings from other authors were confirmed. Especially Reynolds number dependency of drag coefficients and the strong influence of transonic regime were highlighted.
<table>
<thead>
<tr>
<th>Study</th>
<th>Approach</th>
<th>Ma range</th>
<th>Re range</th>
</tr>
</thead>
<tbody>
<tr>
<td>BAILEY and HIATT [15, 16]</td>
<td>experimental, free-flow</td>
<td>0.10 - 6.00</td>
<td>10 - 100,000</td>
</tr>
<tr>
<td>CHARTERS and THOMAS [35]</td>
<td>experimental, free-flow</td>
<td>0.29 - 3.96</td>
<td>93,000 - 1,300,000</td>
</tr>
<tr>
<td>CROWE [40]</td>
<td>theoretical</td>
<td>0.05 - 2.00</td>
<td>0.1 - 1,000</td>
</tr>
<tr>
<td>HENDERSON [81]</td>
<td>theoretical</td>
<td>0.01 - 6.00</td>
<td>1 - 250,000</td>
</tr>
<tr>
<td>HODGES [86]</td>
<td>experiment, free-flow</td>
<td>2.20 - 9.70</td>
<td>n.a.</td>
</tr>
<tr>
<td>KANE [97]</td>
<td>experimental, wind-channel</td>
<td>2.10 - 2.80</td>
<td>15 - 800</td>
</tr>
<tr>
<td>NAGATA et al. [135]</td>
<td>numerical DNS, free-flow</td>
<td>0.20 - 2.00</td>
<td>300</td>
</tr>
<tr>
<td>YUJUAN et al. [211]</td>
<td>numerical IBM, free-flow</td>
<td>1.16 - 2.81</td>
<td>n.a.</td>
</tr>
</tbody>
</table>

**Table 4.2.:** Overview of studies considered for particle drag coefficient improvement in supersonic flows.
CHARTERS and THOMAS [35] presented experimental measurement of drag coefficients for spherical particles in a wide range of free flow Mach and at high Reynolds numbers. They found a strong increase in the value in transonic regime $0.5 < Ma < 1.4$. Particle Reynolds number was found to have an insignificant influence on the drag coefficient in supersonic regime, however lowering the Reynolds number increased drag coefficients in transonic regime significantly.

CROWE [40] gave a comprehensive overview of possible drag coefficient formulations for spherical particles in supersonic flows and took into account various Mach and Reynolds number regimes as well as particle and gas temperatures. He compared various correlations to experimental data and concluded that for low Mach numbers increasing Reynolds numbers lead to decreasing drag coefficients. For higher Mach numbers these differences become smaller but are still detectable.

HENDERSON [81] reported a new correlation for the drag coefficient of spheres incorporating particle and fluid temperatures. The novelty about this formulation was stated to be its validity throughout the subcritical Reynolds number range (i.e. $0.1 < Re_p < 250,000$) and Mach numbers up to 6. Henderson confirmed this validity by means of a comparison study to experimental and theoretical data from literature.

HODGES [86] published an experimental study on drag coefficients of spheres in high Mach number free-flows. He found a constant negative slope of the drag coefficients in the range of Mach numbers from 2 to 4 decreasing the sphere’s drag coefficient from 0.40 to 0.36 followed by a constant value of 0.36 in higher Mach number ranges until $Ma = 9.7$.

KANE [97] experimentally investigated drag coefficients of spheres at high Mach and low Reynolds numbers in a wind-tunnel and found neither a significant influence of Mach numbers nor of particle diameters on drag coefficients in the ranges investigated. The author compared his findings to subsonic data from literature and confirmed smaller drag coefficients for constant Reynolds numbers in subsonic flows compared to supersonic flows in the range of higher Reynolds numbers (i.e. $Re_p > 100$) and vice versa for lower Reynolds numbers.
NAGATA et al. [135] published a numerical study for various Mach and low Reynolds number regimes of rotating and non-rotating spheres. They investigated flow patterns and pressure fields around the spheres in detail and found non-rotating spheres in subsonic conditions to establish a non-uniform downstream flow field and it appeared to become uniform in supersonic conditions.

A strong increase of drag coefficients was reported comparing subsonic to supersonic data. Pressure contributions were reported to have a more significant influence on drag coefficients compared to viscous contributors. The significance of particle rotation was found to be more important in weak flows (i.e. low Mach numbers) compared to stronger flows (i.e. high Mach numbers). The authors presented a classification map of possible flow fields around spheres subdividing the downstream vortex regimes into 5 sections depending on free flow Mach numbers and particle rotation.

YUJUAN et al. [211] investigated numerically shock cell structures and the density field around stationary and moving cylinders. As a main result, time dependent drag coefficient development was presented for various supersonic cases. An exponential correlation of maximum drag values encountered was presented as a function of Mach number.

Summarizing the above results into schematics of the problems encountered in this work results in Fig. 4.30, which is discussed below.

The schematic shows that the presence of voluminous particles inside convergent divergent nozzles modifies the flow state in a transient manner. Depending on the particle position there might be a shift of the nozzle’s actual throat (S’) and hence the local flow pattern is strongly modified. If the particle is located in the convergent nozzle section (situation 1), the flow is accelerated around the particle and decelerated again in the convergent nozzle part downstream the particle before being accelerated again in the divergent nozzle part.
This leads to local pressure field modifications triggered by the presence of particles influencing fore- and afterbody pressure. The flow is forced towards the particle after passing the temporal throat \( S' \) and therefore flow separation is avoided. These two phenomena increase the particle drag coefficient significantly.

![Diagram](image)

**Figure 4.30.** Schematic from theoretical problem investigation of supersonic particle acceleration flows.

The second theoretical situation shows a particle located in the divergent nozzle part. Here, a shock can form upstream the particle because its velocity may be lower than the air velocity which in this situation is already supersonic. Flow is decelerated around the particle and the shock is reflected at the nozzle walls forcing the flow to expand inside the nozzle.

The above fore- and afterbody pressure effects may establish here also. Shocks and the subsequent patterns of expansion- and compression-waves make the flow regime highly transient and complicated, especially in terms of numerical simulations. It was found that these phenomena in the divergent part of the nozzle do not affect the particle drag coefficient significantly, and this is shown below.
4.5.2 Results

It is possible to estimate actual drag coefficients of all model particles investigated by means of experimental data from the validation experiments (see sections 4.1.2 and 4.2.2) and corresponding steady state numerical simulations of the flow field in the transparent validation nozzle. This re-engineering procedure of determining drag coefficients is described in detail in section A.7 in the Appendix.

![Graph showing experimental drag coefficients as a function of particle Reynolds number for 4 bar (left) and 6 bar (right).](image)

**Figure 4.31.** Experimental drag coefficients as a function of particle Reynolds number, 4 bar (left) and 6 bar (right).

Based on these re-engineered results, experimental drag coefficients are correlated as functions of the particle Reynolds number in Fig. 4.31 and the flow Mach number in Fig. 4.32. A possible formulation of the drag coefficient as a function of Reynolds number leads to ambiguous results but the Mach number turns out to be a usable variable for a new empirical correlation.

Larger particles appear to influence the drag coefficient more significantly compared to smaller particles. However, the trends of drag coefficients seem to be approximately independent from particle size and also from nozzle pressure if expressed as functions of Mach number.
Therefore, the re-engineered data is correlated by means of an exponential fit
\[ c_D(Ma) = K_1 \cdot Ma^{-K_0} \] (4.5)
and corresponding correlation coefficients are found to be only slightly dependent on system pressure (neglecting the particle diameter influences as discussed above).

All coefficients for the cases presented here are summarized in Tab. A.5 in section A.7 in the Appendix. Figure 4.32 contains the correlated trends using Eqn. (4.5) with the mean values from Tab. A.5. Both situations (i.e. 4 bar and 6 bar nozzle pressure) are fitted well with this approach and therefore it is assumed that the mean values are valid for drag coefficient prediction inside this nozzle as long as the flow at the outlet is supersonic.

The new correlation, Eqn. (4.6), was implemented into Ansys CFX by the author and it was necessary to clip the upper and lower bound to experimental data
\[ c_D = \min\{3.50, \max[K_1 \cdot Ma^{-K_0}, 0.39]\} . \] (4.6)
All unsatisfactory simulations were repeated with this modification and this leads to the new results presented in Fig. 4.33 and 4.34 in comparison to the
Figure 4.33.: Results from repeated numerical simulations with modified empirical drag coefficient formulation in comparison to old results and experimental data; 2.5 mm POM particles inside the nozzle operating at 4 bar and 6 bar (left) and POM particles of various sizes at the outlet of the nozzle operating at 8 bar (right).

old results and experimental data. The representative trends for 2.5 mm POM particles are shown in the left-hand display in Fig. 4.33 as a function of the nozzle length for 4 bar and 6 bar nozzle pressure and corresponding trends for the remaining POM particle sizes considered are given in Fig. A.14 in section A.7 in the Appendix.

Figure 4.34.: Results from repeated numerical simulations with modified empirical drag coefficient formulation in comparison to old results and experimental data; dilutely-laden dry-ice flow (left) and densely-laden dry-ice flow (right); nozzle operating at 8 bar.
The right-hand display in Fig. 4.33 shows the mean POM particle velocities at the outlet of the nozzle operating at 8 bar. Figure 4.34 compares dry-ice particle velocities at the nozzle outlet for the dilutely-laden flow (left-hand display) and these for the densely-laden flow (right-hand display) at 8 bar nozzle pressure. A significant improvement of the predictions is achieved in all cases considered and the deviations of the mean particle velocities at the nozzle outlet (i.e. at the relative nozzle length = 1) are minimized.

All these resulting deviations are assessed in Tab. 4.3 and most of the deviations are almost bi-sected by the new correlation. However, a pressure and particle size dependency (see also section A.7 in the Appendix) is still visible in the new results. The deviations of the predictions increase with increasing operating pressure and with increasing particle size.

<table>
<thead>
<tr>
<th>Case</th>
<th>Old deviations, sim. with Eqn. (2.68)</th>
<th>New deviations, sim. with Eqn. (4.6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 bar, POM</td>
<td>5.1 %</td>
<td>2.4 %</td>
</tr>
<tr>
<td>6 bar, POM</td>
<td>9.7 %</td>
<td>6.9 %</td>
</tr>
<tr>
<td>8 bar, POM</td>
<td>23.7 %</td>
<td>12.5 %</td>
</tr>
<tr>
<td>8 bar, dry-ice, dilute</td>
<td>20.5 %</td>
<td>8.4 %</td>
</tr>
<tr>
<td>8 bar, dry-ice, dense</td>
<td>35.3 %</td>
<td>23.1 %</td>
</tr>
</tbody>
</table>

**Table 4.3:** Comparison of mean velocity deviations between numerical and experimental data at the outlet of the nozzle for all cases considered.

The validity of this new approach is limited to the nozzle geometry and pressure settings investigated and it is used for steady state simulations independent of the particle loading and the particle size. To generalize the above findings and to add physical meaning to the modified drag coefficient formulations for convergent divergent nozzle simulations in high-pressure flows, extensive additional work is necessary. This necessity is addressed in detail in the summary in Chapter 9. However, the weaknesses of the original numerical toolbox utilized for the dry-ice nozzle simulations in conjunction with compressible flows have been successfully minimized.
5 Particle breakup modelling

This chapter deals with the development of a novel particle breakup model for numerical simulations of CO$_2$ dry-ice impact breakage in Lagrangian particle tracking applications. The procedure presented is mainly influenced by the most extensive investigations towards dry-ice by KRIEG [103], REDEKER [156] and HABERLAND [72] and the most recent water-ice particle breakup studies by HAUK et al. [77, 78], VARGAS et al. [200] and those from PAN and RENDER [143, 158] and GUEGAN et al. [69, 70]. The literature survey for the particle breakup model was presented in Chapter 3.

The particle breakup process is governed by an overall energy balance of the impacting particles, which is initially described in section 5.1. A theoretical model derivation is given in section 5.2 and it is followed by a sensitivity analysis which is used to identify most important contributors to the breakup process and to simplify the physical description. Section 5.2 contains all relevant information which is necessary to close the derived energy balance (for example the literature related derivation of internal bond energy for CO$_2$ dry-ice).

A fundamental HSC experiment is presented in section 5.3, where single dry-ice particles are recorded while impacting solid walls at a range of impact velocities, angles and wall temperatures. The data acquired from post-processing of these recordings represents the statistical database for the new particle-breakup model. Section 5.3 contains detailed information about the linking between post-processed data and final database, which is underpins the new particle breakup model.

The modelling assumption used is comparable to what was introduced and applied by CHAPELLE et al. [32, 33, 34] as a breakup model for industrial granules, although the model presented here uses an energy balance as its fundamental formulation and single particle observations as its fundamental dataset.
Representative single particle data as well as total results are presented in the last part of section 5.3 and the dry-ice breakup process is discussed.

Finally, a Matlab model is developed in section 5.4, which is based on the above theoretical formulation in conjunction with experimental data. This model is described in detail and all necessary assumptions are highlighted. Total results from sample computations are discussed. The model's implementation into Ansys CFX is briefly described and a verification study and a comparison study between original model and Ansys CFX implementation are presented. The verification study shows good agreement between the model outcomes and the basic experimental model data.

5.1 General problem description

Initial HSC experiments on the behaviour of CO₂ dry-ice particles impacting solid walls at impact velocities in the range expected in commercial aircraft defouling applications revealed that the particles tend to disintegrate into secondary particles rather than to directly sublime or melt (which was reported e.g. by HABERLAND [72] for significantly higher impact velocities). Such a disintegration process is shown in Fig. 5.1 for a dry-ice particle impacting a solid wall at approximately 15 m/s impact velocity and an impact angle of approximately 20° (measured from wall's normal direction).

Based on these initial experiments it is concluded that the particle breakup process is not negligible in simulations of indirect cleaning processes such as

**Figure 5.1:** Initial HSC recording of single dry-ice particle (primary particle) impacting a solid wall (at the left-hand side) and disintegrating into smaller fragments (secondary particles).
aircraft engine compressor cleaning, which is addressed here. However, no such breakup models are currently available for Euler-Lagrange particle simulations in Ansys CFX and no appropriate particle breakup model is reported in the literature for CO\textsubscript{2} dry-ice to date (see Chapters 1 and 3). A schematic of the model assumption used in this work is shown in Fig. 5.2.

**Figure 5.2.** Schematic of primary particle impact and breakup process with secondary particle rebound.

The impacting particle can be seen to enter a control volume (red square, in a numerical simulation for example the first cell next to the wall) with the velocity \( \vec{v}_p \). The surrounding fluid (here air) is moving at the velocity \( \vec{u}_{air} \). There is a distance \( \delta x \) between particle and target until final contact and the fouled target is assumed to be potentially moving with the velocity \( \vec{v}_{tar} \) (i.e. a rotor blade of an axial aircraft compressor) and to have the temperature \( T_{tar} \).

Particle material properties are represented by vector \( \psi_p \) and the particle has a certain size \( d_p \) and temperature \( T_p \) and it moves at a certain level \( z_p \) above a reference height. The center image of Fig. 5.2 shows this primary particle on impact. A portion of the fouling is removed from the target (\( \delta m_{fou} \) in the right-hand scheme of Fig. 5.2) and the primary particle disintegrates upon wall contact into secondary particles. A certain proportion of mass, \( \delta m_{sub} \), is sublimated. After this impact (right-hand side of Fig. 5.2), secondary particles \( i \) of various sizes are reflected from the wall at various velocities.
5.2 Theoretical model development

In this section the above particle breakup process (Fig. 5.2) is mathematically formulated. A set of equations is derived and sensitivity analysis is applied to simplify the model using variable values from commercial aircraft engine cleaning. This simplified formulation is used in the later simulations to predict impact breakup of dry-ice particles.

5.2.1 Basic formulation

Applying an energy balance to the impact process described above (Fig. 5.2) leads to the following formulation:

\[
E_{P,\text{kin}} + E_{P,\text{pot}} + E_{P,\text{th}} + E_{\text{air}} = \sum_{i=1}^{n} \left( E_{i,\text{kin}} + E_{i,\text{pot}} + E_{i,\text{th}} + E_{i,\text{air}} \right) + E_{\text{sub}} + E_{\text{er}} + E_{\text{diss}}
\]  

(5.1)

where single energy contributions are written in a general notation (i.e. \( E \) = energy). The left-hand side of Eqn. (5.1) describes the energy of a single impacting particle from the initial moment of observation until the moment of impact. The right-hand side represents the energies of \( i = 1 \ldots n \) rebounded secondary particles after primary particle disintegration. Amounts of further energy proportions from impact and erosion are considered in additional terms (here sublimation, erosion and dissipation).

All single contributions to Eqn. (5.1) are written in detail as follows, assuming all particles to be ideal spheres. The particle mass is

\[
m_p = \rho_p \cdot \frac{\pi}{6} d_p^3
\]  

(5.2)

where \( \rho_p \) is the particle’s density. Its mass moment of inertia is

\[
\theta_p = \frac{2}{5} m_p \cdot \frac{d_p^2}{4}
\]  

(5.3)
Kinetic energy is calculated using Eqn. (5.2) and (5.3)

\[ E_{P,\text{kin}} = \frac{1}{2} \left( m_p \cdot \vec{v}_p^2 + \theta_p \cdot \vec{\omega}_p^2 \right) \]  

(5.4)

accounting for translational and rotational components with the rotational frequency \( \vec{\omega} \). In the potential energy contribution, particle elevation (here represented by z-coordinate) is considered:

\[ E_{P,\text{pot}} = m_p \cdot z \cdot \vec{g} \]  

(5.5)

and \( \vec{g} \) is the acceleration due to gravity. Thermal energy

\[ E_{P,\text{th}} = m_p \cdot c_p \cdot T_p \]  

(5.6)

incorporates the particle’s specific heat capacity \( c_p \) and temperature. The last portion of energy on the left-hand side of Eqn. (5.1) is an assumption concerning the energetic drag contributions from surrounding continuum (in this case air). The signum function is used to determine increase or decrease of particle energy depending on the direction of air velocity:

\[ E_{\text{air}} = c_D \cdot \frac{\rho_{\text{air}}}{2} \cdot \text{sig} \left[ \vec{u}_{\text{air}} - \vec{v}_p \right] \cdot (\vec{u}_{\text{air}} - \vec{v}_p)^2 \cdot A_{p,\text{proj}} \cdot \delta \text{x}. \]  

(5.7)

The variable \( c_D \) describes the drag coefficient (see Sections 2.1.2 and 4.5) and \( A_{p,\text{proj}} \) is the projected area of the particle.

The first four contributions above are also applied to the secondary particles, which can be seen on the right-hand side of Eqn. (5.1). These are calculated from Eqn. (5.2) to (5.7) and must be considered for all secondary particles \( i \). The amount of energy to release one secondary particle from the primary particle’s structure is

\[ E_{i,\text{bu}} = \gamma_i^{[0]} \cdot A_i^{[0]} \]  

(5.8)

with \( \gamma_i^{[0]} \) representing specific surface energy of the particle (i.e. bond energy) and \( A_i^{[0]} \) representing the surface area of totally broken bonds. The amount of
energy necessary for sublimation of a certain portion of particle mass during impact is

\[ E_{\text{sub}} = \delta m_{\text{sub}} \cdot \delta h_{pc} \]  

(5.9)

and \( \delta h_{pc} \) is the specific phase-change (index \( pc \)) enthalpy of this particle. The amount of energy consumed for erosion of a proportion of target’s coating layer (i.e. fouling) can be expressed by

\[ E_{er} = \delta m_{fou} \cdot e_{fou}^{\{er\}} \]  

(5.10)

where \( e_{fou}^{\{er\}} \) is specific erosive energy of the fouling material which is for example related to the defouled proportion of mass. The above energy balance, Eqn. (5.1), requires the balancing of all masses involved in the particle breakup process. The overall mass balance is therefore written as

\[ m_p = \sum_{i=1}^{n} m_i + \delta m_{\text{sub}}. \]  

(5.11)

### 5.2.2 Simplification and closure

In order to simplify the describing set of equations for breakup modelling, single contributors to the above energy balance, Eqn. (5.1), are tested in terms of sensitivity to the application case. The impact of all possible energy contributors is related to primary particle kinetic energy, which is not negligible in this dynamic process, and these energy quotients are used to simplify the set of equations. If a proportion considered is is low enough (i.e. lower than 10 %), its contribution is neglected in the simulation procedure. This sensitivity analysis is described in detail in section B.1 in the Appendix.

Furthermore, a theoretical derivation of the internal bond energy (i.e. \( \gamma^{[0]} \)) of dry-ice particles is presented in section B.2 in the Appendix. With this derivation
the breakup energy proportion, which represents the amount of breakup energy necessary for the breakup of one single secondary particle from impinging primary particles, can be described

\[ E_{i, bu} = \gamma^{[0]} \cdot C_{A, bu} \cdot d_i^2. \]  \hspace{1cm} (5.12)

and the model constants \( \gamma^{[0]} = 0.095 \, J/m^2 \) and \( C_{A, bu} = 0.242 \) are used assuming dry-ice manufacturing pressure to be \( p_{man} = 100 \, bar \) and utilizing the derived Young’s modulus for dry-ice \( Y_{co2} = 1.395 \, GPa \) (see section B.2 in Appendix).

A summary of the sensitivity analysis to the basic energy balance, Eqn. (5.1) is given in Tab. B.1 in section B.1 in the Appendix and it is based on the application case considered in this study. All the coefficients used, equations of the coefficients, critical variables used, maximum error estimates and the final decision as to whether or not the energy contributor is negligible are presented.

The study reveals that breakup and sublimation energy are not negligible in the range of variables considered. Furthermore, defouling erosion energy is only negligible if the amount of energy necessary to defoul a certain proportion of the substrate is small enough. This energy proportion is not known a-priori and therefore it is adressed in Chapter 6 of this study.

Referencing the above sensitivity analysis and resulting parameter study, it is concluded that from the original energy formulation, Eqn. (5.1), potential, thermal and aerodynamic work contributions can be neglected in the description of the impact process addressed here. Dissipative energy is assumed to be contained in the amount of breakup energy and it is therefore also neglected. The final simplified energy balance is written as follows:

\[ E_{P,kin} = \sum_{i=1}^{n} \left( E_{i,kin} + E_{i, bu} \right) + E_{sub} + E_{er} \]  \hspace{1cm} (5.13)
5.3 Experimental investigation

This part of the study was supported by ZITZMANN, T.-A. [IV] and his work was supervised by the author.

Breakup behaviour of dry-ice particles upon impact on solid walls is expected to be comparable to what is summarized in section 3.3 from several water-ice impact studies. A schematic of the process assumption is presented in Fig. 5.2. In this section, a HSC experiment is described which is set up to elaborate statistical data for the above particle breakup balancing equations, Eqn. (5.11) and (B.9). The test rig and the data acquisition procedure are described in detail in the first part of this section. The second part presents an overview of overall experimental results for impact induced particle breakup behaviour of dry-ice.

5.3.1 Set-up

An unfouled (i.e. clean) target is considered for the basic observations of the dry-ice particle breakup processes. Erosive energy contributions to Eqn. (B.9) are neglected because no erosion of the target material is expected. Following these assumptions, the energy balance of an unfouled system, considering particle breakup and possible sublimation on particle-wall collision, is explicitly written as:

\[
\frac{1}{2} \cdot m_p \cdot \vec{v}_p^2 = \sum_{i=1}^{n} \left[ \frac{1}{2} \cdot m_i \cdot \vec{v}_i^2 + \gamma^{[0]} \cdot A_i \right] + \delta m_{sub} \cdot \delta h_{pc} \quad (5.14)
\]

and the corresponding mass balance is given as:

\[
\rho_p \cdot \frac{\pi}{6} \cdot d_p^3 = \sum_{i=1}^{n} \left[ \rho_i \cdot \frac{\pi}{6} \cdot d_i^3 \right] + \delta m_{sub} \quad (5.15)
\]

where the particle masses \( m_i \) are derived from Eqn. (5.2). The variables \( n, m_i \) (represented by \( \rho_i \) and \( d_i \)), \( \vec{v}_i \) and \( \delta m_{sub} \) must be determined from experimental recordings using an appropriate post-processing strategy and statistical
data processing methods. All material properties and dry-ice temperature are assumed to be constant. Physical uncertainties for these model assumptions are:

- slightly sub-cooled dry-ice particle temperatures remain neglected because the process is treated as approximately isothermal with $T_{pc} \approx -78.5^\circ C$ following KRIEG [103]

- internal bond energy is estimated with the procedure presented in section B.1 in the Appendix (i.e. Eqn. (B.18), (B.22) and (B.7))

- dry-ice particle density is assumed to be constant for all particle sizes, with a mean value calculated from the upper and lower bounds presented by HABERLAND [72]: $\rho_i \approx 1420 \, \text{kg/m}^3$

Single dry-ice particles are made to impact a solid target of various temperatures in a range of particle sizes, velocities and impact angles in order to derive the above unknown variables of the breakup process for Eqn. (5.14) and (5.15). The pre- and post-impact data of these particles is recorded by means of HSCs and it is post-processed with the methods described and assessed in Chapter 4.

In section A.1 in the Appendix, the procedure for primary particle tracking is described by Eqn. (A.2) to (A.5) and in section A.5 in the Appendix the procedure for particle sizing is described by Eqn. (A.7) to (A.14). Secondary particles are not tracked individually. Instead, outer bounds of secondary particle clouds are tracked in 3D along the target plate and in horizontal direction in relation to the primary particle impact point (see section 3.5).

Statistical procedures are used to generate a database for the balancing equations from the raw recordings. Assuming $\chi$ to be the replacement character for variables $n, m_i$ and $|\vec{v}_i|$, general statistical relations

$$\chi = f\left[p^{\{x\}}\right] \quad (5.16)$$

are assumed to be valid. In conjunction with experimental derivations of mean values $\bar{\chi}$ and scattering $\chi^\prime$, the specific probability of occurrence $p^{\{x\}}$ from
Eqn. (5.16) is modelled with a given distribution function (here for example a standard distribution, as described in [26])

\[ p\{x\} = \frac{1}{\sqrt{2\cdot\pi\cdot\chi'}} \cdot \exp \left[ -\frac{1}{2} \cdot \left( \frac{x - \chi}{\chi'} \right)^2 \right]. \]  

(5.17)

Various statistical fits can be considered, depending on the experimental results, changing this expression. General functional relations are expected to be found from experimental data

\[ \chi, \chi' = f \left[ d_p, \vec{v}_p, T_{tar} \right]. \]  

(5.18)

It is assumed that particle size (in terms of equivalent spherical diameters \(d_p\)), particle velocity \(\vec{v}_p\) and target temperature \(T_{tar}\) are possible variables in the breakup process and therefore they have to be varied in the experiments. Final variables of secondary particles from primary particle breakup can be calculated

\[ \chi = \chi_d \left( d_p, \vec{v}_p, T_{tar} \right) + \xi_{[i\rightarrow j]} \cdot \chi' \left( d_p, \vec{v}_p, T_{tar} \right) \]  

(5.19)

and the statistical manner of the breakup process is considered by scaling case-dependent fluctuations \(\chi'\) with an appropriate random number \(\xi\) which is varied from \(i\) to \(j\).

A gas-gun acceleration system, shown in Fig. 5.3, is used in order to generate single particle impacts. Particles (8) are accelerated by a compressed air driven piston (6) through the acceleration cylinder (1). The piston (6) is decelerated by compressed air damping at the end of the stroke (7) and particles (8) are made to impact the target plate (2). This target plate (2) can be heated or cooled by means of a temperature management system (4).

This system is shown in detailed section views in Fig. 5.4. Two 50 W load resistors (8) are used to heat the target above ambient temperatures. A Peltier element (10) can optionally be mounted in order to cool the target plate below ambient temperatures. In this case, the heat is removed by an ethanol-fed cooling circuit (11). The temperature management system is controlled by a
Figure 5.3.: Experimental set-up for single particle impact testing, overview (left) and details of particle ejection and end-of-stroke damping (right); CAD model by ZITZMANN [IV].

Figure 5.4.: Detailed section view of target heating device (left) and cooling device (right); CAD model by ZITZMANN [IV].
PID regulator and the preselected temperature is measured by a PT100 thermocouple (9), which is placed in the middle of the target plate $250\mu m$ below its surface.

The impact angle is adjustable by turning the target, Pos. (5) in Fig. 5.3. There is a black background screen mounted around the target (3) to obtain a strong contrast for HSC recordings of impacting dry-ice particles. These are loaded manually into the piston (6), as they are thermoactive and brittle and tend to sublimate or disintegrate before being made to impact the target if not handled carefully while loading. These problems have also been reported elsewhere [156].

For the same reasons, secondary particles can only be collected and measured or weighed within a short period of time after primary particle impact. Secondary impacts can cause further damage and small particles can sublimate and both situations would distort the actual results. Therefore, an experimental set-up was selected which allows live observation of the impact process from two HSCs. This set-up is shown in Fig. 5.5. It is comparable to that reported by VARGAS et al. in [200] for single water-ice particle impact studies.

**Figure 5.5:** Snapshot of experimental set-up with HSCs #1 and #2 mounted around accelerator and target.
HSC #1 records primary particles along their paths from the accelerator's end-of-stroke to the target plate. From these recordings, primary particles are sized and tracked and data relevant to the right-hand side of Eqn. (5.14) and (5.15) is determined. The field of view of HSC #2 is redirected to the target by an adjustable mirror because secondary particles are expected to be distributed in 2D along the target plate (based on the state-of-the-art review and preliminary tests). This phenomenon was also observed for water-ice particles by various authors (see section 3.3).

An example from preliminary tests with dry-ice particles can be seen in Fig. 5.6. Images of a 1200 µm dry-ice particle made by HSC #1 are shown. This particle is impacting the target in normal direction (i.e. 0° impact angle measured to the target's normal direction) at approximately 35 m/s. In the left-hand image of Fig. 5.6 the primary particle is approaching the target, the middle image shows the instant of impact and the right-hand image shows secondary particles being distributed along the target surface a few time-steps after primary particle impact. The 2D distribution behaviour of secondary particles is clearly visible.

**Figure 5.6.:** Example of dry-ice particle impact at medium velocity (35 m/s) recorded with HSC #1 (side camera).

The range of variations of the experimental set-up are summarized as follows in Tab. 5.1. These are based on preliminary handling tests and under consideration of desired boundaries from the application case.

The lower bound of the particle size range is determined by handling tests, which revealed 250 µm to be the smallest particle size which could be handled manually. The upper bound results from the dimensions of the piston. Impact velocities are determined by air velocities and rotational speeds of the blading.
Table 5.1.: Variable ranges of the set-up of the single dry-ice particle impact experiment.

<table>
<thead>
<tr>
<th>particle size</th>
<th>impact velocity</th>
<th>impact angle</th>
<th>target temp.</th>
<th>cycle time</th>
</tr>
</thead>
<tbody>
<tr>
<td>[µm]</td>
<td>[m/s]</td>
<td>[°]</td>
<td>[°C]</td>
<td>[min]</td>
</tr>
<tr>
<td>250 - 4000</td>
<td>1 - 120</td>
<td>0 - 89</td>
<td>-50 - +250</td>
<td>~2</td>
</tr>
</tbody>
</table>

encountered in the test-engine compressor. Impact angles, all measured from the wall’s normal direction, cover the whole range of possibilities, and target temperature was desired to be adjustable between particle sublimation temperature (to exclude possible thermal effects upon experimental results) and the maximum temperatures encountered in higher compressor stages of the test engine in cleaning mode.

Since a reliable statistical database must be generated, a certain number of single particle recordings is required. Therefore cycle time is an important criterion of the experimental design. Its average value was found to be 2 min to acquire data of one single particle impact.

The frames from HSC #2 are manually preselected before post-processing. Frames must be chosen in which the initial densely-laden cloud of very small dust particles has disappeared and the remaining dispersed particles are spread widely enough across the target plate to be distinguished by post-processing methods. This strategy is commonly used in water-ice impact tests (see section 3.3). A preliminary scene representing development of the dust cloud for dry-ice particle impacts can be seen in Fig. 5.7. The approaching primary particle, shown in the left-hand image, disintegrates initially in the middle image and dust (indicated by the red dashed ellipses) is explosively accelerated away from the impact point.

In the right-hand image of Fig. 5.7 slower secondary particles can be seen spread over the target plate some instants of time after primary impact. These recordings were made during run-up tests of the experiment. Examples of selected HSC #2 frames containing secondary dry-ice particles, which were recorded with final HSC set-up, are shown in Fig. 5.8. The left-hand image shows an example for secondary particles of a low velocity impact of approximately 12 m/s
Figure 5.7.: Dry-ice particle disintegration process recorded by HSC #2 (mirror-observing camera): primary particle (left), initial cloud of dust (center) and larger secondary particles (right).

and the right-hand image shows the same situation for a high speed impact of approximately 100 m/s. Smaller secondary particles can be seen for the high velocity impact compared to its left-hand counterpart. Single secondary particles can be found, counted and sized with the post-processing methodology described in section A.5.

In order to estimate secondary particle post-impact velocities, an elliptical envelope is assumed to contain these particles and the outer bounds of this ellipse are tracked. The envelope is described by the fastest dispersed particles. How-

Figure 5.8.: Secondary dry-ice particles distributed along target plate for low velocity (left) and high velocity (right); impact recorded by HSC #2 (mirror-observing camera).
ever, the initial cloud of dust (see discussion of Fig. 5.7) remains neglected because it disappears form the HSCs field of view directly after impact. The temporal development of the envelope of secondary particles is tracked with both HSC #1 and #2 in relation to the impact piont of the primary particle. This situation is described in more detail and a procedure is presented to derive experimental based ellipse parameters in section B.3 in the Appendix.

These parameters $a$, $b$, $c$ and $a_{ELL}$ are used to describe the envelope of the secondary particle cloud and any secondary particle velocity vector can be modelled using the parametric ellipse equation:

$$
\vec{v}_{p}^{[\text{c,e}]} = \begin{cases} 
\pm a_{ELL} + \xi_{[0\rightarrow1]} \cdot a \cdot \cos(\xi_{[0\rightarrow2]} \cdot \pi) \cdot \cos(\xi_{[0\rightarrow0.5]} \cdot \pi) & \text{...direction } x \\
\xi_{[0\rightarrow1]} \cdot b \cdot \sin(\xi_{[0\rightarrow2]} \cdot \pi) \cdot \cos(\xi_{[0\rightarrow0.5]} \cdot \pi) & \text{...direction } y \\
\xi_{[-1\rightarrow0]} \cdot c \cdot \sin(\xi_{[0\rightarrow0.5]} \cdot \pi) & \text{...direction } z
\end{cases}
$$

(5.20)

where $\xi$ are uniformly distributed random variables and the index in brackets $[i \leftrightarrow j]$ indicates an appropriate range of values.

Results from model calculations with Eqn. (5.20) are illustrated in Fig. 5.9 for various impact angles and secondary particle velocities. Impact points are located at the graph’s origin (i.e. (0,0)).

Secondary particle envelopes can be seen in 2D along the target surface at certain instants of time after primary particle impact. The left-hand graph is calculated with a mid-point velocity of the ellipse lower than its spreading velocity (i.e. $a_{ELL} < a/2$) and the right-hand graph shows a situation where $a_{ELL} > a/2$.

The final choice of the important HSC settings field of view, spatial and temporal discretization is a compromising decision between precision and reproducibility of the recordings as well as manageability of the experiment. Important uncertainties from the set-up apply to secondary particle numbers and sizes. Since secondary particles are detectable only after the initial cloud of dust disappears and after dispersed secondary fragments are far enough distributed to be clearly distinguishable, a certain proportion of primary particle mass and hence a number of secondary particles is lost in the post-processing.
The sensor size of HSC #2 is chosen in preliminary tests to be large enough to record at least three frames per impact showing most of the secondary particles. These must be spread widely enough on the recordings to be clearly post-processible. Sizing of detected secondary particles is done in 2D and mirror-dependent field of view deteriorations are considered. These lead to local differences in spatial discretization up to 15%. Furthermore the 2D assumption leads to possible sizing uncertainties of up to 15 % with respect to the diameter, which was estimated in pre-tests with non-spherical POM particles. The smallest particle size detectable is limited by the spatial discretization. All HSC settings chosen are summarized for the main dry-ice impact testing in Tab. 5.2.

<table>
<thead>
<tr>
<th>HSC</th>
<th>field of view [px x px]</th>
<th>spatial discretization [px/mm]</th>
<th>temporal discretization [fps]</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1</td>
<td>768 x 248</td>
<td>30</td>
<td>20,025.6</td>
</tr>
<tr>
<td>#2</td>
<td>384 x 396</td>
<td>14 - 17</td>
<td>20,025.6</td>
</tr>
</tbody>
</table>

**Table 5.2.**: Final HSC settings for dry-ice impact experiment to the new particle breakup model.
5.3.2 Results

A preliminary study of the above test-rig revealed the particle velocity - pressure relation displayed in Fig. 5.10. Particle velocity is correlated with a logarithmic fit based on a total number of 630 POM particle tracks (diameter: 1.5 mm) which were accelerated using operating pressures from 0.1 to 2.3 bar.

At higher pressure levels (2.5 to 5.0 bar) this correlation is checked with 60 additional POM tracks of the same particle size and these datapoints are not considered in the correlation. It can be seen that the accuracy of reproducibility of the particle emission velocity is approximately +/-10 %. The logarithmic correlation presented is used to preselect emission velocity of the set-up in the later experiments with dry-ice.

The experimental database must be dependent on particle impact velocity, impact angle and target temperature, which is discussed in Sections 5.2 and 5.3.1. Dry-ice particle size cannot be controlled exactly in the tests presented here because it is not possible to produce single dry-ice particles of a certain size and of material properties comparable to original pellets. Hence, original dry-ice pellets are initially disintegrated (which is known to happen in dry-ice blasting machines, see section 4.3 for details), and the fragment particles produced,

![Graph showing particle velocity as a function of system pressure](image)

**Figure 5.10.** Particle emission velocity as a function of system pressure, experimental results from 1.5 mm POM particles and logarithmic correlation.
which are assumed to enter aircraft engines for cleaning purposes, are used as primary particles for the impact tests presented.

Parameter values for the basic experiment are chosen as listed below:

- particle impact velocities (nominal): 6, 12, 25, 50, 100 m/s
- particle impact angles: 0°, 20°, 40°, 60°
- target temperatures: -20, 0, 20, 40, 80°C

This listing is based on further run-up studies with the test-rig and estimated bounds from the application case. The lower temperature bound is the lowest ambient temperature expected in actual engine wash situations. Tests at lower temperatures cannot be made without significantly increasing the cycle time of the experiment (see Tab. 5.1) mainly due to rapid freezing of the target from ambient humidity.

A total of 3,800 single dry-ice particles were shot with the above parameters to acquire a statistically reliable database for the new breakup model. The number of particles to be shot for each parameter setting was dependent from the availability of the HSC equipment and the manpower which was necessary to conduct this lengthy experiment. Given the desired number of parameters to be investigated (i.e. 5 velocities, 4 angles and 5 target temperatures resulting in 100 parameter combinations) and the pre-estimated cycle time for single particle impact acquisition (~2 min.) as well as set-up times etc. a total of 36 particles was pre-defined to be shot for each parameter.

Some additional tests were made at the outer boundaries of the experiment (i.e. lowest and highest temperature and angle in combination with all velocities). High velocity tests turned out to be most challenging because numerous primary particles disintegrated in the piston prior to firing. In these cases, multiple fragments impacted the target and the acquired data was removed from post-processing.

Some representative results of impact tests are shown in Fig. 5.11 to 5.15. There is a comparison shown in Fig. 5.11 between secondary particle distributions from low impact velocity (i.e. 6 m/s, left-hand graph) and high impact velocity (i.e. 100 m/s, right-hand graph). High velocity impacts produce finer secondary
Figure 5.11.: Secondary particle size distributions for normal impacts upon heated target (80°C) for low impact velocity (6 m/s, left) and high impact velocity (100 m/s, right).

particles compared to low velocity impacts (also compare e.g. to Fig. 5.8). The same situation is shown in Fig. 5.12 using the Gates-Gaudin-Schumann nomenclature encountered in some publications by THRONTON et al. [96, 125, 181].

Secondary particle size distributions from all single particle impacts (blue x-marked trends) are displayed for both above velocities (left-hand display: 6 m/s

Figure 5.12.: Secondary particle size distributions for normal impacts upon heated target (80°C) for low impact velocity (6 m/s, left) and high impact velocity (100 m/s, right) in GGS terminology.
and right-hand display: 100 m/s) in one graph with corresponding mean distributions estimated from all single particle trends (red o-marked trends in both graphs). The larger scattering of secondary particle sizes encountered for the low impact velocities is clearly visible from the left-hand side graph. There are single impacts producing only a couple of dust and being disintegrated into a low number of fragments carrying a large proportion of primary particle mass. This situation is not observed for high velocity impacts, even if there are some single secondary particles carrying more than 10% of the primary particle mass.

An example for secondary particle velocities encountered is given in Fig. 5.13. Envelopes of secondary particle distributions can be seen for a given instant of time after primary particle impact. The impact point is centered to the graph’s origin (i.e. (0,0)). All secondary particle envelopes are plotted along the target surface (i.e. in 2D, blue ellipses) and their mid-points as well as the displacement vectors related to the impact point are shown as black circles and coloured lines respectively.

For the normal impacts displayed in Fig. 5.13, there is no predominant midpoint velocity direction detectable. Higher secondary particle velocities resulting from higher impact velocities (i.e. 100 m/s) form larger ellipsoids.

**Figure 5.13:** Secondary particle envelopes at the same instant of time after normal impact at heated target (80°C) for low (left, 12 m/s) and high impact velocity (right, 100 m/s).
(Fig. 5.13, right) compared to their counterparts from lower impact velocity (i.e. 12 m/s shown in Fig. 5.13, left).

Figure 5.14 shows a significant change in secondary particle's ellipsoid formation and displacement from the impact position if impact angle increases. The right-hand graph in Fig. 5.13 shows the situation of high velocity impact normal to the wall (i.e. impact angle 0°) and Fig. 5.14 contains ellipsoids for the same impact velocity but 60° impact angle. The impact position is shifted in this graph to the right to make it comparable to above Fig. 5.13, right.

![Diagram of ellipsoids](image)

**Figure 5.14.:** Secondary particle envelopes at a certain instant of time after high velocity (100 m/s) impact at heated target (80°C) with high impact angle (60°).

Next, experimental results are tested for possible correlations to primary particle diameter and, if possible, the data is normalized by the latter. The least squares method, described for example in [26], is used to correlate experimental outcomes (here generally represented by $\chi$) as linear function of primary particle diameter $d_i$. This is done by minimizing the squared residual $\mathbb{R}_{tot}^2$ of each such possible data correlation:

$$
\sum_{i=1}^{m} \{ \chi_i - (C_1 \cdot d_i + C_0) \}^2 = \min \{ \mathbb{R}_{tot}^2 \} \quad (5.21)
$$
and variable $m$ represents the number of primary particle impacts considered. With final correlation functions from Eqn. (5.21), coefficients of determination $R^2_x$ are calculated to evaluate the strength of possible correlations:

$$R^2_x = \frac{\sum_{i=1}^{m} \left\{ (\tilde{C}_i \cdot d_i + \tilde{C}_0) - \bar{x} \right\}^2}{\sum_{i=1}^{m} \left\{ x_i - \bar{x} \right\}^2} = \frac{\sigma^2_{cor}}{\sigma^2_x}. \quad (5.22)$$

It represents the quotient of the variance covered by the regression function $\sigma^2_{cor}$ related to the real variance encountered in measured data $\sigma^2_x$. Examples for experimental datasets are shown in Fig. 5.15 and these have various correlation strengths. The number of secondary particles is plotted against the primary particle diameter for a range of primary particle impacts at 6 m/s in the left-hand graph of Fig. 5.15. The right-hand graph shows the same situation for primary particle impacts at 25 m/s. A linear dependence on the number of secondary particles produced by higher impact velocities is clearly visible, but there is no such dependence detectable from low velocity impacts.

An analysis of all data acquired in the main tests using the method outlined above reveals the results presented in Fig. 5.16. Mean correlation strength is classified as significant if $R^2_x \geq 0.33$, which is the case for the number of

![Figure 5.15: Example from correlation testing: number of secondary particles from low (6 m/s, left) and medium impact velocity (25 m/s, right) as a possible function of primary particle diameter.](image-url)
secondary particles and for the diameter of dispersed secondary particles for all nominal impact velocities despite the lowest.

Secondary particle velocity does not correlate significantly with primary particle diameters for all nominal primary particle velocities considered. Based on this analysis, number and diameters of secondary particles are related to primary particle diameter in what follows. No such relation is considered for secondary particle velocities.

The main experimental results are discussed in Fig. 5.17 to 5.20. Figure 5.17, left, shows related numbers of secondary particles against all impact velocities considered and various impact angles. Volume-related primary particle kinetic energy is used for the abscissa, which here is a function of velocity only hence dry-ice density is assumed to be constant. The same variables are shown in the right-hand display but impact angle is kept constant and target temperature is varied. These global trends show that there is an influence of the impact angle upon the number of secondary particles (i.e. the number decreases with increasing impact angle) and there is no clear difference encountered for temperature variations. However, there seems to be a damping effect from highly sub-cooled or superheated targets compared to the remaining data, which is most clearly developed for highest impact energies.

Figure 5.16.: Correlation tests of secondary particle values as a function of primary particle diameter.
Figure 5.17.: Number of secondary particles (related to the primary particle diameter) as a function of impact energy for various impact angles (left) and target temperatures (right).

In Fig. 5.18 the above parameters are discussed for related secondary particle diameters of the debris particles. An influence of the impact angle can be seen in the left-hand graph for low impact energies, where increasing debris diameters are detectable for increasing impact angles. This influence becomes smaller when impact energy is increased. This influence could not be detected for residual particles (not shown here). In the right-hand graph, there is no influence visible from target temperature variations, secondary particle sizes appear to be a function of primary particle kinetic energy and impact angle only.

Figure 5.18.: Diameter of secondary particles (related to the primary particle diameter) as a function of impact energy for various impact angles (left) and target temperatures (right).
In a third comparison, secondary particle mean post-impact velocities are discussed as a function of impact angle (Fig. 5.19, left) and target temperature (Fig. 5.19, right). There is no clear angle influence visible for low impact energy, however, an influence is detectable for higher energy values in Fig. 5.19 left, and the secondary particle velocity increases with increasing impact angles.

The secondary velocity also seems to be independent from target temperature when the impact energy is low (Fig. 5.19, right). However, there is a lower secondary particle velocity detectable for low target temperatures and it becomes more significant with increasing impact energy. This may be attributed to secondary velocity damping influenced by the presence of a thin frost layer on target surface from ambient humidity, which could not be avoided totally during the experiments.

**Figure 5.19.**: Mean velocity of secondary particles as a function of impact energy for various impact angles (left) and target temperatures (right).

Impacts upon targets at ambient temperature (i.e. 20°C) and upon moderately super-heated targets (i.e. 40°C) produce most secondary particles and highest secondary particle velocities, which can be seen in Fig. 5.17 and 5.19 respectively. A stronger super-heating or sub-cooling of the target damps secondary particle production and velocities. The strongest sub-cooling (i.e. -20°C) significantly limits the number and velocities of secondary particles and the strongest super-heating (80°C) significantly reduces the number of secondary particles.
Figure 5.20: Mean coefficients of restitution as a function of target temperature and impact angle.
This damping can be attributed to convective air flow in case of super-heated targets and potential ice layer build-up on targets in sub-cooled cases.

Finally, representative results for mean normal and tangential coefficients of restitution are shown in Fig. 5.20 for all parameters tested at one impact velocity. The left-hand graph of Fig. 5.20 shows normal coefficients of restitution (i.e. mean normal secondary particle velocity related to primary particle velocity) plotted as a function of target temperature and impact angle. The above angle dependence can clearly be seen and no temperature dependence is visible. The right-hand graph of Fig. 5.20 shows tangential coefficients of restitution as a function of the same two variables. A clear influence of the impact angle and a slight dependence on target temperature can be seen. The tangential coefficient of restitution decreases slightly with decreasing target temperature. Tangential coefficients of restitution greater than unity are possible, because secondary particle interaction during impact causes the 2D distribution of the secondary particles described above even if the primary particle hits the target in normal direction.

The tangential coefficients of restitution cannot be computed for normal primary particle impacts because in this case the denominator of Eqn. (3.3) would be zero. Therefore, the right-hand graph of Fig. (5.20) starts at an impact angle of 20°. It can be shown formally that the mass- and energy conservative particle breakup model presented here also satisfies momentum conservation and this proof is presented in Appendix B.4.

5.3.3 Development of breakup criterion

This part of the study was supported by: LUONG, H. [V] and his work was supervised by the author.

It was necessary to develop a physical decision criterion to determine the onset of particle breakup of dry-ice particles. This necessity is based on observations made during the main experiment. These show that some of the low velocity impacts produce only a low number of small secondary fragments and one major secondary particle of a size comparable to the primary particle. This
indicates a change of fragmentation mode dependent on impact variables. Many authors already addressed various fragmentation modes of disintegrating particles, which is summarized in section 3.3. An example of such a situation for dry-ice is shown in Fig. 5.21. Both stills show secondary dry-ice particles after impact. The left-hand display shows minor fragmentation and the right-hand image shows major fragmentation.

It is important to create a boundary function to distinguish between these fragmentation modes. Preliminary tests into dry-ice fragmentation behaviour show that there is minimum minor fragmentation encountered in the range of dry-ice diameters and impact velocities addressed within this work. This boundary function serves as decision criterion as to whether an impacting particle should be disintegrated or not in later numerical simulations, where minor fragmentation is treated as non-fragmentation mode.

For the above purpose, HAUK’s breakup boundary function presented in [77, 78] is used. It is presented in Eqn. (3.2) and can explicitly be expressed as correlation between normal impact velocity, primary particle diameter and a correlation coefficient $\alpha$:

$$
\nu_p^{(n)} = d_p^{[i]} \cdot d_p^{\left(-\frac{2}{3}\right)}.
$$

This correlation coefficient is dependent on particle material and the breakup-modes to be distinguished, which are indicated by the superscript $\{i\}$.

To experimentally underpin the above relation for the boundary description of minor and major fragmentations of dry-ice, an appropriate correlation coefficient
Particle size | Impact velocity | Impact angle | Target temp. | Cycle time
---|---|---|---|---
[µm] | [m/s] | [°] | [°C] | [min]
250 - 4000 | 0.5 - 9.0 | 0 | 20 | ~2

Table 5.3.: Experimental parameters of additional tests into dry-ice breakup modes.

must be found. Therefore, an additional set of simplified impact investigations is recorded. The experimental set-up presented in section 5.3.1, Fig. 5.3 to 5.5, is used and only HSC #1 is applied to observe the scene from the side. A representative recording is shown in Fig. 5.21. The range of this additional study is small compared to the main experiment and the parameters are summarized in Tab. 5.3.

Only normal impacts at ambient temperature are considered to generate the data necessary to fit the above function. Initially, these results presented below are assumed to be valid for the whole parameter range of the main experiment. Future work is necessary to prove this assumption or to adjust the data.

In order to automatically post-process the experimental data, various breakup criteria were tested, from which

\[
b_u = \frac{n_{p2}}{d_{p2}} \left( \frac{\max[d_{p2}]}{d_{p1}} \right)^2
\]  \hspace{1cm} (5.24)

turned out to be the most reliable. It relates the number of secondary particles encountered in the recordings to the square of the quotient of maximum secondary particle diameter and primary particle diameter. An appropriate threshold value \(bu_{tr,v} = 20\) was found in a comparison study between manually post-processed experimental samples and automatically post-processed samples. The final breakup indicator for dry-ice was found to be

\[
BU = \begin{cases} 
1 & \text{if } bu \geq bu_{tr,v} \\
0 & \text{if } bu < bu_{tr,v}
\end{cases}
\]  \hspace{1cm} (5.25)
Figure 5.22.: Breakup modes as a function of primary particle diameter and velocity, dry-ice (left) and water-ice from HAUK [78] (right).

where major breakups are indicated as ones and minor breakups as zeros. An error estimation revealed false indications in 5% of the cases, which was deemed to be acceptable.

A total of 200 samples was recorded and automatically post-processed and the final results are shown in Fig. 5.22. The related correlation coefficients are summarized in Tab. 5.4.

The left-hand graph shows main results for dry-ice indicating minor and major breakups and the correlated boundary. There is a mixed mode zone detected, where minor and major breakups can occur. It is assumed that there is a second boundary between this mixed mode and major disintegration mode but this was not investigated within this work. The mixed mode can be attributed to

<table>
<thead>
<tr>
<th>particles</th>
<th>boundary</th>
<th>coefficient $\alpha \left[ \frac{m^2}{s} \right]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>dry-ice</td>
<td>no - minor</td>
<td>n.a.</td>
</tr>
<tr>
<td></td>
<td>minor - major</td>
<td>0.074</td>
</tr>
<tr>
<td>water-ice [78]</td>
<td>no - minor</td>
<td>0.046</td>
</tr>
<tr>
<td></td>
<td>minor - major</td>
<td>0.140</td>
</tr>
</tbody>
</table>

Table 5.4.: Correlation coefficients for fragmentation mode boundaries of dry-ice and water-ice.
the manufacturing process of dry-ice pellets, in which dry-ice snow is pressed. The resulting pellets are of inhomogenous and brittle structure.

On the right-hand side of Fig. 5.22 a sample of the data presented by HAUK in [78] is shown for comparison of dry-ice to water-ice. The boundary distinguishing between minor and major breakup for water-ice is higher than this for dry-ice, which can be attributed to lower density and a more stable crystalline structure of water-ice particles compared to pressed dry-ice. HAUK et al. also reported a boundary correlation between no and minor breakup. The elaboration of this boundary was not possible for dry-ice. Furthermore, no mixed mode zone was reported for water-ice.

5.4 Numerical model development

This part of the study was supported by LUONG, H. [V] and by REIS, P. [VI] and their work was supervised by the author.

In this section, the breakup model development in Matlab is described in detail. Representative computational results are presented and discussed. Furthermore, the implementation of the Matlab based breakup model into Ansys CFX is described, initial simulation results are shown and implementation-related differences between the original model and the Ansys CFX implementation are stressed.

5.4.1 Set-up

Initially, a classification of secondary particle sizes must be introduced for the particle breakup model. Its purpose is to account for all experimental limitations reported in section 5.3.1. Generally following THRONTON et al. [96, 125, 181, 192, 193], a mass fraction dependent differentiation between large and mean particle sizes is applied. This classification is complemented by experimental restrictions and an overview of particle size classes applied to the model is given in Tab. 5.5.

In order to describe the lower bound of residue particles (denoted by res), a mass fraction value of 10 % is utilized following [96, 125, 181, 192, 193].
<table>
<thead>
<tr>
<th>Description</th>
<th>Size-Class</th>
<th>Mass-Fraction Range</th>
<th>Mean Diameter</th>
<th>Data Origin</th>
</tr>
</thead>
<tbody>
<tr>
<td>large</td>
<td>res</td>
<td>$\frac{m_{res}(d_P)}{m_P} &gt; 0.1$</td>
<td>variable</td>
<td>main experiment</td>
</tr>
<tr>
<td>mean</td>
<td>deb</td>
<td>$0.1 &gt; \frac{m_{deb}(d_P)}{m_P} &gt; m_{deb} (d_P = 80\mu m)$</td>
<td>variable</td>
<td>main experiment</td>
</tr>
<tr>
<td>small</td>
<td>dust</td>
<td>$m_{dust} (d_P = 80\mu m) &gt; \frac{m_{dust}(d_P)}{m_P} &gt; m_{dust} (d_P = 20\mu m)$</td>
<td>38.67\mu m</td>
<td>special experiment</td>
</tr>
<tr>
<td>very small</td>
<td>cont</td>
<td>$m_{cont} (d_P = 20\mu m) &gt; \frac{m_{cont}(d_P)}{m_P} &gt; m_{cont} (d_P = 564\text{pm})$</td>
<td>15.67\mu m</td>
<td>assumption</td>
</tr>
</tbody>
</table>

**Table 5.5.** Particle size classes used in the new particle breakup model.
The lower bound for debris particles (denoted by deb) arises from the smallest secondary particle size detectible in the main HSC experiments, which is approximately $80 \, \mu m$. This value depends on the spatial discretization of the field of view of HSC #2. Smaller particles (i.e. dust) must be distinguished into particles which potentially contribute to defouling action (denoted by dust) and particles, which do not contribute to defouling (denoted by cont).

Following [27, 28, 104, 105, 116, 117, 118], the critical particle size for erosion is reported to be in the range from 10 to $20 \, \mu m$. However, the lower value cannot be adapted for the lower bound of dust particles, because the smallest particle size detectible with the above HSCs in a special purpose experimental set-up to measure the dust class (described further below) is $20 \, \mu m$. Therefore, particles smaller than $20 \, \mu m$ are treated as irrelevant to defouling erosion and are considered to belong to the above very small continuous size class. The diameters of these particles are assumed to range from $20 \, \mu m$ to $536 \, pm$ (i.e. dry-ice molecules according to [43]).

The particle size distributions of residue and debris particles are derived from experimental data (basically described by Eqn. (5.17)). The distribution of dust particle sizes is investigated in a special purpose experiment, where a reduced number of primary particle breakups was investigated with the maximum possible spatial discretization of HSC #2 in the same way as described in section 5.3.1. With these results, statistical dust particle sizes are defined

$$d_{dust} \approx 38.67 \pm 11.16 \, [\mu m] \, .$$

(5.26)

The distribution of continuous particles is derived by mass averaging between the maximum particle diameter of the continuous phase (i.e. $d_p = 20 \, \mu m$) and a single dry-ice molecule (i.e. $d_p = 536 \, pm$):

$$\bar{d}_{cont} = \left( \frac{d_{dust,min}^3 + d_{mol}^3}{2} \right)^{\frac{1}{3}} \approx 15.87 \, [\mu m] \, .$$

(5.27)
Consideration of the above particle size classification leads to modifications of the basic energy and mass balances applied, Eqn. (5.14) and (5.15). The energy balance is rewritten under consideration of the above particle size classes:

\[ E_{\text{P,kin}} = \sum_{i=1}^{n_{\text{res}}} (E_{i,\text{kin}} + E_{i,\text{bu}}) + \sum_{j=1}^{n_{\text{deb}}} (E_{j,\text{kin}} + E_{j,\text{bu}}) + (E_{\text{dust,kin}} + E_{\text{dust,bu}}) + (E_{\text{cont,kin}} + E_{\text{cont,bu}}) + E_{\text{sub}} \]  

(5.28)

where residue and debris particles are treated as individual dispersed particles. Mean particle sizes according Eqn. (5.26) and (5.27) are applied to all dust and continuous particles respectively. These phases are accelerated to the maximum post-impact envelope velocity in the simulations and this approach is assumed to be valid based on the qualitative observations of post-impact behaviour of the cloud of dust (see above discussion of Fig. (5.7)).

Similar modification of the mass balance leads to:

\[ m_{\text{P}} = \sum_{i=1}^{n_{\text{res}}} m_{i} + \sum_{j=1}^{n_{\text{deb}}} m_{j} + \delta m_{\text{dust}} + \delta m_{\text{cont}} + \delta m_{\text{sub}} \cdot d_{\text{P}} \]  

(5.29)

With the above experimental results, Eqn. (5.19) to (B.28), single proportions of energy and mass can be calculated for Eqn. (5.28) and (5.29) and this is described below. The procedure represents the core module of the particle breakup model.

Debris class contributions are balanced starting with the number of debris particles (note that only integers are allowed)

\[ n_{\text{deb}} = \left\lfloor \left( \bar{n}_{\text{deb}}^{*\{\text{EX}P\}} + \bar{\xi}_{[-1\longleftrightarrow+1]} \cdot \bar{n}_{\text{deb}}^{*\{\text{EX}P\}} \right) \cdot d_{\text{P}} \right\rfloor \]  

(5.30)

followed by the corresponding particle sizes of \( i \) debris particles (for the present with \( C_{\text{corr}} = 1 \))

\[ d_{i,\text{deb}} = \left( \bar{d}_{\text{deb}}^{*\{\text{EX}P\}} + \bar{\xi}_{[-1\longleftrightarrow+1]} \cdot \bar{d}_{\text{deb}}^{*\{\text{EX}P\}} \right) \cdot d_{\text{P}} \cdot C_{\text{corr}}^{\frac{1}{2}} \]  

(5.31)
and the total particle mass

\[ \delta m_{deb} = \sum_{i=1}^{n_{deb}} \left( \frac{\pi}{6} \cdot \rho_p \cdot d_{i,deb}^3 \right). \] (5.32)

In the second step, residual particle mass is calculated

\[ \delta m_{res} = \left( p_{m,(res+deb)}^{[EXP]} \cdot m_p \right) - \delta m_{deb} \] (5.33)

by means of experimentally investigated mass proportion of dispersed residue and debris particles related to the primary particle mass

\[ p_{m,(res+deb)}^{[EXP]} = \frac{\delta m_{res}^{[EXP]} + \delta m_{deb}^{[EXP]}}{m_p^{[EXP]}}. \] (5.34)

After this, residue particle size is set according to experimental values (here only mean values are considered and for the present \( C_{corr} = 1 \))

\[ d_{i,res} = \bar{d}_{res}^{[EXP]} \cdot d_{P} \cdot \bar{C}_{corr}^{\frac{1}{3}} \] (5.35)

and the number of residue particles is calculated from the mass balance

\[ n_{res} = \left[ \frac{\delta m_{res}}{\frac{\pi}{6} \cdot \rho_p \cdot d_{i,res}^3} \right]. \] (5.36)

Because, as above, only integer values are allowed for the number of residual particles, the mass balance is not necessarily satisfied by the above procedure. Therefore, a correction factor is applied to the residue particle diameter, Eqn. (5.35):

\[ C_{corr} = \frac{\left( p_{m,(res+deb)}^{[EXP]} \cdot m_p \right)}{\sum_{i=1}^{n_{deb}} m_{i,deb} + \sum_{j=1}^{n_{res}} m_{i,res}}. \] (5.37)
and Eqn. (5.35) and (5.36) are recalculated. If, after the correction of the
residue class, there is still a correction necessary to satisfy the overall mass
balance (i.e. $C_{corr} \neq 1$), a second correction loop is applied to debris particle
sizes, Eqn. (5.31), which finally enforces mass conservation. This correction
procedure turns out to generate maximum deviations of +/-10% for residue
particle sizes and +/-1% for debris particle sizes which is explicitly stressed in
the discussion of Fig. 5.34 (verification study below, section 5.4.4).

The accumulated mass of dust particles is calculated with

$$\delta m_{dust} = (1 - p_{sub}) \cdot \left(1 - p^{[EXP]}_{m,(res+deb)}\right) \cdot p^{[EXP]}_{m,dust} \cdot m_p \quad (5.38)$$

where $p^{[EXP]}_{m,dust}$ is the dispersed dust particles mass proportion related to the ac-
cumulated remaining primary particle mass (i.e. $\left(1 - p^{[EXP]}_{m,(res+deb)}\right) \cdot m_p$). This
value is derived from additional high-precision experiments concerning the dust
class:

$$p^{[EXP]}_{m,dust} = 0.0375. \quad (5.39)$$

The variable $p_{sub}$, which represents the proportion of primary particle mass
actually sublimated, is estimated by an iterative closure procedure. This pro-
cedure is based on closure of the model related energy balance. To keep the
describing Eqn. (5.41) and (5.42) shorter, a replacement mass proportion

$$\delta m_{ADD} = \delta m_{dust} + \delta m_{cont} + \delta m_{sub} = \left(1 - p^{[EXP]}_{m,(res+deb)}\right) \cdot m_p \quad (5.40)$$

is introduced, which represents all masses related to small particle size classes
(i.e. dust, continuous and sublimated). For the same reason a replacement
particle size $d_{ADD}$ is incorporated.

With these values, an overall energy balance can be written:

$$\frac{1}{2} \cdot m_p \cdot \vec{v}_p^2 = \sum_{i=1}^{n} \left[ \frac{1}{2} \cdot m_i \cdot \vec{v}_i^2 + \gamma^{(0)} \cdot A_i \right] + \delta m_{ADD} \cdot \left[ \left(1 - p_{sub}\right) \cdot \left(\frac{1}{2} \cdot \vec{\rho}_{ADD}^2 + \frac{6}{\pi} \cdot \frac{C_{Ahu}}{d_{ADD} \cdot \rho_p} \right) + p_{sub} \cdot \delta h_{pc}\right] \quad (5.41)$$
where the only unknown variable is the sublimated proportion of mass $p_{sub}$. Rearrangement of Eqn. (5.41) leads to an iteration rule

$$
p_{sub} = \left\{ \frac{1}{2} \cdot m_p \cdot \bar{v}_i^2 - \left[ \sum_{i=1}^{n} \left( \frac{1}{2} \cdot m_i \cdot \bar{v}_i^2 + \gamma^{(i)} \cdot \bar{A}_i \right) + \delta m_{add} \cdot (1 - p_{sub}) \right] \cdot \left( \frac{1}{2} \cdot C_{add} \cdot \bar{v}_p + \frac{6}{\delta \bar{h}_{pc}} \cdot \bar{A}_i \right) \right\} \cdot \frac{1}{\delta m_{add} \cdot \delta h_p}, \tag{5.42}
$$

from which the unknown variable $p_{sub}$ can be calculated by a simple iteration procedure

$$\frac{LHS\left(p_{sub}\right)}{RHS\left(1 - p_{sub}\right)} < 10^{-5} \tag{5.43}$$

which relates the left-hand side $LHS$ of Eqn. (5.42) to the right-hand side $RHS$ of Eqn. (5.42).

With $p_{sub}$, the total mass of dust particles is calculated with Eqn. (5.38). The number of dust particles is estimated with a mass balance relation and the mean dust diameter from Eqn. (5.26):

$$n_{dust} = \left[ \frac{\delta m_{dust}}{\frac{\pi}{6} \cdot \rho_p \cdot d_{dust}^3} \right]. \tag{5.44}
$$

Finally, the total mass of continuous secondary particles

$$\delta m_{cont} = \left(1 - p_{sub}\right) \cdot \left(1 - p_{m, (res + deb)}^{\{EXP\}}\right) \cdot \left(1 - p_{m, dust}^{\{EXP\}}\right) \cdot m_p \tag{5.45}
$$

and the sublimated proportion of primary particle mass

$$\delta m_{sub} = p_{sub} \cdot \left(1 - p_{m, (res + deb)}^{\{EXP\}}\right) \cdot m_p \tag{5.46}
$$

are calculated.

Conservation of energy is achieved by calculation of kinetic energy proportions for all secondary particles, which is done individually for residue and debris particles only. Mean values are applied for dust and continuous particles.

$$E_{kin, i} = \frac{m_i}{2} \cdot \bar{v}_i^2 \left( d_P, v_P, \alpha_{IMP}, T_{tar} \right) \tag{5.47}$$
The velocity vector is estimated with Eqn. (5.20). Furthermore, all breakup energy proportions

\[ E_{bu,i} = \gamma^{[0]} \cdot C_{A,bu} \cdot d_{pi}^2 \]  

(5.48)

are calculated from Eqn. (B.18), (B.22) and (B.23). Finally, the proportion of sublimation energy is determined

\[ E_{sub} = \delta h_{PC} \cdot m^{[SUB]} \].  

(5.49)

The above procedure satisfies the overall mass balance of the particle breakup

\[ m_p \overset{!}{=} \delta m_{res} + \delta m_{deb} + \delta m_{dust} + \delta m_{cont} + \delta m_{sub} \]  

(5.50)

and the overall energy balance

\[ E_{p,kin} = \sum_{i=1}^{n_{ALL}} E_{kin,i} + \sum_{j=1}^{n_{ALL}} E_{bu,j} + E_{sub}. \]  

(5.51)

Momentum conservation is implicitly achieved, and the corresponding mathematical proof of this is presented in section B.4 in the Appendix.

A schematic of the Matlab implementation of the above calculation procedure, Eqn. (5.26) to (5.49), is shown in Fig. 5.23. The equations introduced are referenced in this schematic and all variables are abbreviated. The breakup indicator used, i.e. the determining criterion as to whether particle breakup occurs or not, is introduced in section 5.3.3, Eqn. (5.23).
**Figure 5.23.** Schematic of the computational particle breakup procedure.
5.4.2 Results

Results from dry-ice particle breakup predictions by means of the above computational procedure are shown in Fig. 5.24 to 5.28. Absolute numbers of dispersed secondary particles (residue and debris) are plotted in Fig. 5.24 as functions of volume related kinetic energy of impacting particles for various impact angles. The left-hand graph shows results for low target temperature (i.e. -20°C) and the right-hand graph contains computed results for high temperature target impacts (i.e. +80°C). It can be seen from both graphs that the number of secondary particles increases if the impact angle decreases (i.e. normal impacts produce most secondary particles). This can also be seen from Fig. 5.17, where experimental results are discussed as a function of both impact angle and target temperature.

![Figure 5.24](image)

**Figure 5.24.** Computed number of secondary particles (residue and debris) as a function of impact energy for cold (-20°C, left) and warm (+80°C, left) target.

Figure 5.25 shows computed results for mean secondary particle diameters. There is a slight dependence from the impact angle detectible for both low (left-hand graph) and high (right-hand graph) target temperatures in a certain range of impact energies. At higher target temperature this dependence is less clearly visible compared to low target temperature impacts. The most significant dependence can be seen for low impact velocities at both target temperatures. This result is also comparable to corresponding experimental results, which are discussed in Fig. 5.18. Furthermore, the computations pre-
dict an unbroken rebound in the case of the steepest target angle and lowest impact energy and this can be seen from both graphs Fig. 5.24 and 5.25 (i.e. only one secondary particle is produced and it is significantly larger compared to the other secondary particles).

Mean secondary particle velocities appear to be dependent on impact angle and target temperature and this dependence becomes more significant when the impact energy increases, which is shown in Fig. 5.26.

Figure 5.26.: Computed mean velocity of secondary particles (residue and debris) as a function of impact energy for cold (-20°C, left) and warm (+80°C, left) target.
Figure 5.27.: Example for computed secondary particle velocity vectors and stochastic distribution inside the predicted envelope in 2D.

The left-hand graph shows computed results for low target temperature (i.e. -20°C) and the right-hand graph those for high target temperature (i.e. +80°C). An increase can be seen in secondary particle velocity for increasing impact angles and target temperature. The results are comparable to the discussions of experimental results in Fig. 5.19.

Finally, Fig. 5.27 and 5.28 contain a representation of the secondary particle velocity distribution discussed above and described and computed with Eqn. (5.20). Secondary particle velocity vectors are shown as coloured lines. They all originate at the impact point, which is set to be the origin of the graphs (i.e. (0,0)).

Figure 5.28.: Example situation from Fig. 5.27 in 3D.
Figure 5.27 displays a 2D view of the situation at 1s after impact. The same situation is plotted in Fig. 5.28 in 3D. All secondary particles can be seen to be stochastically distributed inside the elliptical envelope. The normal velocity component is an order of magnitude lower compared to tangential components (note: axis ticks in Fig. 5.27 and 5.28 are not equal for presentation reasons). This result clearly indicates the 2D behaviour of the secondary particles after breakup and highlights its adaption to the new model.

### 5.4.3 Implementation into Ansys CFX

The computational procedure presented in section 5.4.1 and shown schematically in Fig. 5.23 was implemented into Ansys CFX (note that this was done by Ansys developers). This section stresses main differences between the original model and its Ansys implementation.

For this purpose, the number loading of one representative model particle of a certain size class \( \lambda_{cf,x} \) (where the superscript \{CLASS\} represents the actual size class) must be introduced:

\[
\lambda_{cfx}^{\{CLASS\}} = \frac{n^{\{CLASS\}}}{n_{cfx}}.
\]  

(5.52)

It incorporates the quotient between the actual number of particles of the corresponding particle size class from the particle breakup model \( n \) (i.e. CLASS = residue, debris etc.) and the number of numerical model particles representing this particle size class in CFX simulations \( n_{cfx} \). If the number of model particles is one, which means that the particular size class is represented by exactly one model particle, the number loading of this model particle equals the actual number of particles from the original breakup model.

The breakup procedure implemented into Ansys CFX is slightly different to that described in section 5.4.1. These differences are in the diameter correction procedure for residue particles, Eqn. (5.35) and (5.37) and in the determination of the number of debris particles, Eqn. (5.30). There is no diameter correction applied in Ansys CFX and conservation of mass, Eqn. (5.50), and energy,
Eqn. (5.51), is ensured by calculating the numbers of all secondary particles as a result of corresponding mass balances:

\[
\hat{n}_{\text{CLASS}} = \frac{\hat{n}_{\text{CLASS}}^{\text{P}}}{\hat{n}_{\text{CLASS}}^{\text{P}}} = p_{\text{CLASS}}^{\text{P}} \cdot \left( \frac{d_{\text{CLASS}}}{d_{\text{CLASS}}^{\text{P}}} \right)^{3},
\]  

(5.53)

Therefore, any possible differences between computed and experimental results are shifted from the diameter (original particle breakup model) to the number of secondary particles (Ansys CFX implementation). As can be seen from Eqn. (5.53), Ansys CFX utilizes number rate (see section A.6, Eqn. (A.24)) instead of real particle count.

Assuming one model particle per particle size class in Eqn. (5.52) and (5.53) (i.e. \( \lambda_{\text{CLASS}}^{\text{P}} = \hat{n}_{\text{CLASS}}^{\text{P}} \)) the number of secondary particles of a certain particle class can be calculated in Ansys CFX simulations using the quotient of model particle number rate to primary particle number rate (superscript: \( \{P\} \)). This procedure is described in Eqn. (5.53). It can be also expressed by the mass fraction of the corresponding particle size class, which is also shown in Eqn. (5.53). This procedure is comparable to Eqn. (5.36) and (5.44) describing the original model.

The experiment described in section 5.3.1 is turned into an Ansys CFX simulation set-up to perform a run-up and verification study of the breakup model implementation and this is mainly described in the following section 5.4.4. The numerical set-up is shown in Fig. 5.29. Primary particles are made to impact the target without consideration of surrounding fluids. All relevant variables (i.e. primary particle diameter, particle velocity, impact angle and target temperature) can be parametrized in a manner which corresponds to the experiment.

A representative result from such simulations is shown in Fig. 5.30. The left-hand plot shows a high velocity primary particle (red) impacting a target (transparent - light grey) in normal direction at 100 m/s. It disintegrates into 100 model particles on impact. These dispersed secondary particles of size classes residue, debris and dust are shown at a certain instant of time after impact. The left-hand colour map describes particle sizes. The secondary particle’s
Figure 5.29.: Set-up of breakup simulation in Lagrangian particle tracking formulation in Ansys CFX.

The ellipsoid is visible from displayed positions of secondary particles and from particle tracks, which are coloured corresponding to absolute velocity values (without colour map).

The middle image of Fig. 5.30 shows the same situation as described above but simulated with just 3 secondary model particles (i.e. one representing each dispersed particle class). The oversimplification of the actual situation becomes clear when comparing the middle image to its left-hand side counter-

Figure 5.30.: Particle breakup simulation in Lagrangian particle tracking formulation with Ansys CFX, normal impact of a 1 mm dry-ice particle at 100 m/s, various simulation settings.
part. Number rates of the simulation with only 3 secondary model particles are shown in the right-hand side graph of Fig. 5.30. Particles are coloured by their number rate and colours are specified in the right-hand side colour map. Primary particle impact produces predominantly debris particles, second most dust particles and least residue particles in this case.

5.4.4 Verification study

A verification study for the particle breakup model presented in section 5.4.1 and a comparison study between the original model and the Ansys CFX implementation, described in section 5.4.3, is presented here.

To assess the functionality of the model, the main secondary particle properties number, mean diameter and mean velocity (generally represented by $\chi$) of residue and debris particle classes are computed at parameter nodes of the underpinning basic experiment and compared to experimental values by means of the relation:

$$\Lambda_{\chi} = \frac{\chi_{\text{NUM}}}{\chi_{\text{EXP}}}.$$  (5.54)

Some representative results from this verification study are shown in Fig. 5.31 to 5.33. The above relation, Eqn. (5.54), is plotted in Fig. 5.31 left, as a function of target temperature (1st abscissa) and impact angle (2nd abscissa) for low nominal impact velocities of 6 m/s. A systematic underprediction of the number of dispersed secondary particles by approximately 5 % is detected.

This can be explained with the number rounding, Eqn. (5.30), (5.36) and (5.44), and diameter correction procedure, Eqn. (5.35) and (5.37), applied to the particle size classes considered. Since the number of secondary particles at 6 m/s impacts is low compared to high velocity impacts (see Fig. 5.24) a difference of one particle can cause a divergence between computed and experimental values in the order of 10 %. The predicted secondary particle numbers for 100 m/s impacts differ only slightly from corresponding experimental results, which is shown in Fig. 5.31, right. Total assessment of all 100 experimental
Figure 5.31.: Deviations of computations from basic experiment for number of secondary particles at low (6 m/s, left) and high impact velocity (100 m/s, right).

nodes reveals a mean deviation of predicted secondary particle numbers from experimental values of +/-3 %.

The second comparison, Fig. 5.32, deals with mean diameters of secondary particles including residue and debris particle classes. A maximum under-prediction of 5 % can be detected in case of low velocity impact in normal direction and at high target temperature (left-hand graph of Fig. 5.32) and this can be attributed to number rounding and diameter correction as explained in the discussion above. The remaining data appears to reproduce the experimental results with an accuracy of +/-1 %. Total assessment of computational predictions of secondary particle diameters for all 100 experimental nodes re-

Figure 5.32.: Deviations of computations from basic experiment for diameter of secondary particles at low (6 m/s, left) and high impact velocity (100 m/s, right).
A comparison between computed mean secondary particle velocities and corresponding experimental data is shown in Fig. 5.33 for both low and high velocity impacts at all target temperatures and impact angles. These predictions can be seen to be accurate and comparable for both velocities. There is a slight underprediction of the secondary velocities detectable for higher impact angles and both nominal impact velocities. Assessment of the full database reveals a mean deviation of predicted mean secondary particle velocities to experimental values of approximately +/-2 %.

The code is assumed to be verified based on the study presented above. Mean deviations resulting from model assumptions are summarized in Tab. 5.6. The

<table>
<thead>
<tr>
<th>Variable</th>
<th>MAX deviation</th>
<th>MEAN deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{SEK}$</td>
<td>10 %</td>
<td>3 %</td>
</tr>
<tr>
<td>$d_{TOT}$</td>
<td>5 %</td>
<td>2 %</td>
</tr>
<tr>
<td>$v_{SEK}$</td>
<td>3 %</td>
<td>1 %</td>
</tr>
</tbody>
</table>

Table 5.6.: Overview of mean value deviations of numerical to experimental results for breakup model variables.
main reasons for these deviations are found to be the number rounding procedure described in Eqn. (5.30), (5.36) and (5.44) and the enforcement of mass conservation by diameter correction of residue and debris particles by means of Eqn. (5.35) and (5.37). Application of the sublimation assumption, Eqn. (5.41) to (5.43), can also cause deviations since it is not assessed in the experiments.

Finally, a comparison study between the Matlab particle breakup procedure (with superscript hda) and the Ansys CFX implementation (with superscript CFX) is presented in Fig. 5.34 and discussed below. For comparison reasons, quotients of results achieved from application of Eqn. (5.54) for calculations made with CFX and those made with the Matlab model are derived:

\[
Q = \frac{\Lambda^{[\text{CFX}]}_{x}}{\Lambda^{[\text{hda}]}_{x}}. \tag{5.55}
\]

Application of this assessment criterion reveals systematic deviations encountered between computed and experimental values from both codes.

Results are shown in Fig. 5.34, left, for residue secondary particles and in the right-hand display for debris particles. In both graphs results for the number of secondary particles and such for diameter predictions are shown. Several characteristic nodes (i.e. primary particle velocity, impact angle and target temperature) are chosen from the model and the abscissa shows a continuous test number.

Comparable qualitative behaviour of over- or underpredictions from both codes is detected (i.e. quotient values different to unity). If, for example, the hda code is underpredicting the diameter (i.e. a red star-marked nodal value appears to be higher than unity), CFX code is underpredicting the corresponding number (i.e. the blue o-marked nodal counterpart appears to be lower than unity). It is furthermore visible that deviations of predicted diameters of the original model are lower compared to deviations of the numbers of the CFX implementation. This is explainable when taking into account the different mass conservation
Figure 5.34.: Comparison study of CFX particle breakup implementation with original Matlab code by means of Eqn. (5.55), residue size class (left) and debris size class (right).

procedures applied. An exponent of 3 is consequently found to be the exact difference between these deviations, i.e. for the numbers in Fig. 5.34:

\[ \Lambda_n^{[CFX]} = \left( \Lambda_d^{[hda]} \right)^3 \]  
(5.56)

5.5 Summary of particle breakup modelling

A new single particle experiment has been presented to generate breakup statistics for dry-ice particles which are typically used in aircraft defouling applications. The statistical database was analyzed and it was found that the secondary particle number, size and velocity is mainly dependent on the primary particle impact velocity and impact angle. In particular, the number of secondary particles is sensitive to the primary particle diameter but it is not sensitive to the target temperature. The diameters of residual particles were found to be almost independent of impact angle but dependent on primary particle diameter whereas those of debris particles are dependent on the impact angle and almost independent from primary particle diameter. The velocity of secondary particles was found to be dependent on primary particle velocity for low impact
energy and on velocity and impact angle for increasing impact energy. However, additional temperature effects at high impact velocities cannot be ruled out.

Additional experiments have been presented to describe the onset of breakup for dry-ice particles and to determine descriptive statistical properties for very small secondary particles (i.e. dust). The particle breakup is modelled with a mass- and energy-conservative approach and the Matlab implementation of the model was used to simulate typical breakup scenarios. These computed results confirm the secondary particle dependencies discussed above. Furthermore, the Matlab model was implemented into Ansys CFX and both versions were verified against the statistical database underpinning the model. The applied rounding and closure procedures lead to mean deviations for secondary particle properties in the range from 1 % to 3 %. Those maximum deviations encountered with the original Matlab model can be as high as 10 % for the number of secondary particles.

However, it was shown that the Ansys implementation of the model utilizes a different closure procedure and that the predictions of the numbers of secondary particles are less precise in Ansys compared to the original model. The Ansys CFX implementation of the new particle breakup model is used in the validation and in the application case simulations presented in Chapters 7 and 8.
6 Defouling erosion modelling

A part of this study was mainly presented in: RUDEK et al. [VII]

In this chapter a new defouling erosion model is presented, whose general purpose is to account for amorphous, heterogeneous coatings such as those typically found in aircraft compressors. In this work it is applied to the defouling of aircraft engine compressors using dry-ice particles.

The development of a new model is necessary because the corresponding literature review of erosion modelling, which is presented in section 3.4, revealed that no such model is available at present. Following the basic idea of erosion-related energy assessment presented by various authors [90, 91, 92, 101, 102, 145, 147, 148] a “dynamic indentation testing” (DI) experiment is designed which is generally adapted from [91, 92, 184, 194].

Following the basic problem description in section 6.1 and the mathematical formulation of the model in section 6.2, the basic DI experiment is described in section 6.3. This experiment utilizes the set-up presented in the particle breakup model description in section 5.3 but in a partially-modified form. Using this model, particle restitution behaviour is investigated and empirical dissipation and defouling functions are derived.

Non-disintegrating reference material (POM) is used to determine the dissipation energy for defouling action and this idea is based on findings from [18, 42, 63, 64]. These dissipation values are assumed to be specific to the fouling material and valid for indentations of various particle materials and this assumption is based on findings such as those reported in [88, 89, 101, 102] for crystalline materials.

The parameters considered in the experiment are particle impact velocity and angle as well as particle and fouling material. Four typical coatings which are relevant to commercial aircraft defouling processes are investigated. The data acquired represents the statistical database underpinning the new model. It is
possible to enlarge this database to numerous coating and particle materials in the future using the basic experiment presented in this work. Final experimental results are discussed in section 6.3 in terms of defouling efficiency of all material pairings considered.

Based on the above, a Matlab procedure is developed to assess and predict erosive airfoil defouling in terms of defouling functions and to predict the specific energy necessary to remove a certain proportion of fouling. This procedure is described in detail in section 6.4 and typical results from computations are discussed. Furthermore, the Ansys CFX implementation of the model is described and verified and this is also described in the last section 6.4. The verification shows good overall agreement with the statistical database.

6.1 General problem description

The requirements for a new erosion model in the context of aircraft engine defouling are

- to predict defouling indentations precisely and
- to assess the energy consumed in order to indent a particular coating.

A modelling concept is developed based on these requirements, and it is shown schematically in Fig. 6.1. The scheme shows a particle made from a certain material (here represented by the density) and of a certain size (here represented by the diameter) on impact upon a fouled target. This particle impacts the wall with a certain impact velocity $v_{p1}$ and, at a later instant of time, it is reflected from the wall with a certain reflection velocity $v_{p2} < v_{p1}$.

Following the findings from [18, 42, 63, 64, 184, 194], the kinetic energy lost by the particle on impact appears in several forms post-impact. These are described by the variable $\delta e$ in Fig. 6.1. The first proportion which must be considered is dissipation inside the particle (index: $P$), the second is energy consumed to indent and to penetrate through the coating, thickness $\mu$ (index: $f ou$), and the third proportion is used to remove a certain volume of the coating.
Figure 6.1.: Schematic of primary particle impact, defouling and rebound process highlighting the energy based assumption.

(index: \( ER \)). It is assumed that the target material plays a negligible role in this energy balance and the validity of this assumption is adopted from [184, 194].

The particle’s coefficient of restitution (see Eqn. (3.3), here \( \epsilon \)) can be measured and used to determine the sum of these energy proportions (see Fig. 6.1). Further possible energy contributions, such as thermal or potential energy, are assumed to be negligible in this process based on the simplification procedure applied to the particle breakup model described in section B.1 in the Appendix.

The particles used for the above analysis must not disintegrate on impact, and therefore it is necessary to use particles made from reference material instead of dry-ice. The results from reference material testing are scaled by a function to predict the defouling energy of disintegrative materials (i.e. dry-ice) and this function results from comparison of the defouled areas from both particle materials. It is based on the assumption that the defouling energy is specific to the fouling material. The defouled areas are measured in various indentation experiments and they are represented by the diameter of indentation \( d_{IMP} \) in Fig. 6.1.
6.2 Theoretical model development

In this section the model assumption is developed into a statistically-based mathematical model. The whole procedure is described in detail and links from the theoretical formulation to the underpinning experiment are highlighted. Furthermore, a method is introduced to account for non-spherical indentations from dry-ice particles in computational defouling predictions.

6.2.1 Basic formulation

It is assumed that the dependence of restitution coefficients on the Stokes number, such as reported by BARNOCKY and DAVIS [18, 42] and later by GONDRET et al. [63, 64], is valid for the situations investigated. Gondret et al. demonstrated that there is a significant similarity of the restitution process of various particle and surface material combinations in various fluids and this can be described by a single normalized restitution curve. This finding is based on extensive experimental data. The variable for this particular restitution function is the near-wall Stokes number (for details see Eqn. (3.10) and related discussion)

\[ St = \left( \frac{1}{9} \right) \cdot \frac{\rho_p \cdot v_p \cdot d_p}{\eta_f} \]  

(6.1)

and the coefficients of restitution must be normalized by their particular maxima.

The following formulation is used to describe the energy dissipation of a certain particle on impact upon a fouled target and to assess the proportion of defouling energy, which is necessary to indent and to remove a proportion of fouling:

\[ \delta e_{\{\text{part,fou,\alpha}\}} = \frac{\rho_{\text{ref}}}{2} \cdot \delta e_{\{\text{fou,0}\}} \cdot \left( \nu^1_{\{\text{ref EQ,0}\}} \right)^2 \cdot F_{\text{IMP}}_{\{\text{part,fou,\alpha}\}} \]  

(6.2)

It is adapted from the dynamic hardness definition, Eqn. (3.11), which was originally presented in [184] and used by these authors in [185, 210].

Defouling energy $\delta e$ is related to empirical restitution data from reference particle material impacts and, if necessary, scaled with a defouling relation $F_{IMP}$ to any particle material. The superscript is important to this formulation and it reads as follows:

- $part =$ particle material (i.e. $ref\, EQ =$ reference material at equivalent velocity normal to the wall),
- $fou =$ fouling material,
- $\alpha =$ impact angle (i.e. $0^\circ =$ normal to the wall).

The first term on the right-hand side of Eqn. (6.2) describes reference material dissipation (index: $ref$). It is used to consider the difference of dissipated energy from impacts of a non-disintegrating reference material on clean and fouled targets as follows:

$\delta \epsilon^{\{fou, 0^\circ\}} := \left[ \left( \epsilon^{\{0^\circ\}} \right)^2 - \left( \epsilon^{\{fou, 0^\circ\}} \right)^2 \right] \tag{6.3}$

and $\delta \epsilon$ is defined to be the impact dissipation factor. It is derived from experimental data of reference particle rebounds measured in the normal direction to the wall’s surface (superscript: $0^\circ$). Therefore the normal component of reference material particle impact velocity, which is normalized to a dry-ice equivalent (superscript: $ref\, EQ$) is used in Eqn. (6.2). This dry-ice equivalence is derived from Stokes-number comparison of the investigated particles (here dry-ice) to those made from reference material

$\nu^{\{ref\, EQ, 0^\circ\}} = \left( \frac{\eta^{\{ref\}}}{\eta^{\{part\}}} \right) \cdot \left( \frac{\rho^{\{part\}}}{\rho^{\{ref\}}} \right) \cdot \left( \frac{d^{\{part\}}}{d^{\{ref\}}} \right) \cdot \nu^{\{part, 0^\circ\}}. \tag{6.4}$

The variable $\delta \epsilon$ is assumed to be dependent on fouling material (superscript: $fou$) only.
The second contributor to the right-hand side of Eqn. (6.2), $F_{IMP}$, is the scale function. Its superscript indicates that it is a function of particle material, fouling material and impact angle and it can be written as:

$$F_{IMP}^{\{part,fou,\alpha\}} = \left( \frac{d_{IMP}^{\{part,fou,\alpha\}} \left( \frac{1}{v_1^{\{part\}}} \cdot d_P^{\{part\}} \right)}{d_{IMP}^{\{ref,fou,0^\circ\}} \left( \frac{1}{v_1^{\{ref eq,0^\circ\}}} \cdot d_{IMP}^{\{ref\}} \right)} \right)^2. \quad (6.5)$$

The purpose of this function is to scale the proportion of defouling energy calculated by means of the dissipation factor. This dissipation factor is assumed to be dependent on the removed proportion of fouling from reference material indentations and the function above is used to account for actual proportions of defouling energy consumed to indent the same fouling material by any particle material at any impact angle (enumerator superscript: $part, fou, \alpha$).

Empirical particle defouling functions $d_{IMP}^{\{part,fou,\alpha\}} (v_p)$ are included in Eqn. (6.5) and they describe the diameter of the area defouled related to the impacting particle’s diameter $d_P$. These functions depend on the particle’s absolute impact velocity. It is assumed that the indentations are cylindrical and fouling thickness is negligible, therefore the indentation diameters describe the amount of defouling to a satisfactory extent.

The actual defouled area, $A_{IMP}$, from single particle impacts is consequently calculated:

$$A_{IMP}^{\{part,fou,\alpha\}} = \frac{\pi}{4} \cdot \left[ d_{IMP}^{\{part,fou,\alpha\}} \left( \frac{1}{v_1^{\{part\}}} \cdot d_P^{\{part\}} \right) \right]^2. \quad (6.6)$$

6.2.2 Simplification and closure

Based on the results from defouling experiments (reported in section 6.3) it can be decided whether energy contributions from defouling action, Eqn. (6.2), to the overall particle energy balance on impact, Eqn. (5.13), are negligible or not.
To close the above empirical formulation for defouling energy with experimental data, the following correlation procedure is used

\[
\delta \varepsilon_{\text{fou}} = \begin{cases} 
C_A \{\text{fou}\} & \text{...if } 0 < St \leq St_A \\
C_1 \{\text{fou}\} \cdot \ln(St) + C_0 \{\text{fou}\} & \text{...if } \text{LOGopt} = 1 \\
\sum_{j=0}^{n} C_j \{\text{fou}\} \cdot (St)^j & \text{...if } \text{LOGopt} = 0 \\
C_B \{\text{fou}\} & \text{...if } St_B < St 
\end{cases}
\] (6.7)

and it describes the impact dissipation factor either with a logarithmic (\(\text{LOGopt} = 1\)) or with a polynomial function (\(\text{LOGopt} = 0\)) in a critical range of Stokes numbers (\(St_A < St \leq St_B\)). The choice of the appropriate correlation function depends on the experimental data. The defouling variable is clipped to constant values \(C_A\) and \(C_B\) below and above the critical Stokes number range, and in this study it was found \(C_B = 0\) in all cases investigated. The correlation coefficients \(C_j\) are derived from statistical fitting of the experimental data and this is described in section 6.3.

If defouling energy is negligible to the overall energy balance of the impacting particle, the only formulation necessary to predict defouling is given by Eqn. (6.6). Hence, experimentally based defouling functions must be derived

\[
d_{\text{IMP}}^{\{\text{part,fou,}\alpha}\} = \begin{cases} 
0 & \text{...if } v_1 \leq v_{1,\text{crit}}^{\{\text{part,fou,}\alpha}\} \\
K_1^{\{\text{part,fou,}\alpha}\} \cdot \ln(v_1) + K_0^{\{\text{part,fou,}\alpha}\} & \text{...if } v_1 > v_{1,\text{crit}}^{\{\text{part,fou,}\alpha}\}
\end{cases}
\] (6.8)

and appropriate correlation coefficients \(K_i\) for each particle, fouling and impact angle combination must be elaborated. The critical impact velocity \(v_{1,\text{crit}}^{\{\text{part,fou,}\alpha}\}\) determines the onset of erosion for any particular parameter combination,
which is indicated by its superscript. It corresponds to the Stokes number describing the onset of erosion, which is discussed below.

Because angular impacts (i.e. not perpendicular to the walls surface) produce non-spherical and displaced indentations, an additional formulation must be used to account for this in the model. The procedure for this is described in detail in section C.1 in the Appendix. It applies the elliptical eccentricity of the experimental indentations which uses the two ellipse parameters $a$ and $b$ and which is measured

$$\text{ecc}_{\{\text{part,fou,a}\}} : = \left( \frac{a^2 - b^2}{a^2} \right)^{\frac{1}{2}}.$$

(6.9)

The system of descriptive equations, Eqn. (6.1) to (6.6), is closed by means of the procedure described by Eqn. (6.7) to (6.9) and by Eqn. (C.1) to (C.7). The model can therefore be applied after population of the underpinning statistical database. The necessary experimental framework to achieve this and all relevant results are discussed in the next section.

### 6.3 Experimental investigation

This section comprises a description of the modifications to the basic experimental set-up used in the particle breakup investigations, which is presented in detail in section 5.3. These modifications are necessary to make the test-rig applicable for the data acquisition to the new defouling erosion model. Typical results from the basic experiments are discussed in the second part of this section and these are mainly focussed on the defouling predicted and on the corresponding energy assessment.

The main experiments comprise investigations into four different types of fouling which are:

- PTFE, which is used as indicator coating in compressor cleaning experiments at the test-rig,
- SALT, which is also used in test-rig experiments as an artificial fouling but it can also be found in actually fouled compressors,
• ORIGINAL FOULING 1 (ORIG1), which is a heterogeneous mixture of various substances with a high proportion of carbon and which can be found mainly in front compressor stages and

• ORIGINAL FOULING 2 (ORIG2), which is also a heterogeneous mixture of various substances without a dominant amount of any substance and which is found mainly in rear compressor stages.

The PTFE and SALT layers investigated are prepared artificially and ORIG1 and 2 fouling is investigated with airfoils taken directly from service.

Figure 6.2 highlights the main distinguishing feature between the two original fouling materials. The blade coated with ORIG1 fouling appears to be black and the fouling is viscous. The blade with ORIG2 fouling is red and this fouling material is brittle. These main differences are attributed to higher operational temperature and pressure in rear stages of axial compressors, which make carbon and humidity disappear and which bake the fouling to the blades.

Fouling characteristics for all the above materials have been determined in the laboratories of Lufthansa Technik and are presented with their kind permission in this work. The artificially-coated blades were prepared by the author and the
original parts were taken directly from service of Lufthansa aircraft. A 3D focus variation method was used to determine surface roughness and layer thickness and scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) studies were applied to assess fouling material compositions. The main results from these investigations are summarized in Tab. 6.1.

<table>
<thead>
<tr>
<th>Fouling</th>
<th>Layer Thickness $\mu f_0 [\mu m]$</th>
<th>Roughness $R_a [\mu m]$</th>
<th>Mean C-mass fraction $\frac{mC}{M_{fou}} \cdot 100 [%]$</th>
<th>No. of samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>CLEAN</td>
<td>n.a.</td>
<td>0.199 ± 0.048</td>
<td>n.a.</td>
<td>150</td>
</tr>
<tr>
<td>PTFE</td>
<td>19.22 ± 8.22</td>
<td>2.094 ± 0.303</td>
<td>n.a.</td>
<td>150</td>
</tr>
<tr>
<td>SALT</td>
<td>51.88 ± 33.53</td>
<td>4.271 ± 2.067</td>
<td>n.a.</td>
<td>75</td>
</tr>
<tr>
<td>ORIG1</td>
<td>8.79 ± 2.90</td>
<td>5.151 ± 2.953</td>
<td>28.83</td>
<td>60</td>
</tr>
<tr>
<td>ORIG2</td>
<td>16.05 ± 8.77</td>
<td>7.683 ± 2.219</td>
<td>4.93</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 6.1: Characteristic values of clean and fouled airfoils (investigated in Lufthansa Technik laboratories).

6.3.1 Set-up

The modifications made to the basic particle breakup experiment to make it usable for defouling investigations are:

- the implementation of a before-after impact area recording camera,
- the modification of the target holder with a rapid-fixing mechanism for artificially-fouled targets and
- the implementation of a flexible target-holder for original airfoils.

These modifications are put into practice as is shown in Fig. 6.3 and this is described below.

The before-after impact area recordings are made by means of the “impact area CAM”. Its field of view is redirected via the mirror from below to the target plate surface.
Figure 6.3.: Experimental set-up for defouling data acquisition.

This setting is comparable to the recordings made with HSC#2 in the particle breakup experiments and this is explained in the discussion of Fig. 5.5 in section 5.3.1. An example from such before-after impact recordings is shown in Fig. 6.4. A typical indentation from a single particle impact upon a PTFE coated target is shown.

Figure 6.4.: Example: before-after comparison of indented PTFE coating and post-processed indentation (in the box).
Using digital image processing (as described in section A.5 in the Appendix) both image matrices are filtered and subtracted and this results in a difference matrix

$$I_{\text{diff}} = I_{t2} - I_{t1}$$

(6.10)

which contains the indentation information only (example given in Fig. 6.4). This matrix is binarized, Eqn. (A.11), and the information inside the resulting bounding box is processed to obtain the equivalent indentation diameter, calculated with Eqn. (A.13) and (A.14).

The recordings made with the “particle tracking HSC” are used to track and size particles before and after impact. The post-processing procedures used and the associated uncertainty analysis are described in detail in section A.1 in the Appendix.

Figure 6.5 illustrates a typical impact situation with a reference material particle (here: POM) at very low impact velocity (left display). The right-hand side diagram displays the corresponding post-processing result. Pre- and post-impact velocities are shown as a function of the time-step and these velocities are determined by means of the centroid-matching approach, Eqn. (A.4) and (A.5). The mean velocity values are calculated and multiple time-steps around the

![Figure 6.5: Example: impacting particle (left) and resulting pre- and post impact tracking velocities.](image)

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The mean values are used to calculate the coefficients of restitution of the particles.

The slight variance which is visible in the above pre- and post-impact velocity trends results from the precision of the post-processing approach. It is negligible because it is very small compared to the absolute velocity values investigated (note that the diagram in Fig. 6.5 shows the lowest particle velocity considered). Furthermore, multiple time-steps are used to determine the mean velocity values. The slight slopes of the velocity trends presented in Fig. 6.5 are caused by gravity, which is also assumed to be negligible. It is not considered in post-processing.

The most important statistical values of the main experiments are summarized in Tab. 6.2. There are two impact angles considered at which potential erosion maxima are expected (details are explained in section 3.4). The particle sizes are varied in a range comparable to the particle breakup studies and the target temperature is not parametrized in the defouling tests.

Table 6.3 summarizes the main camera settings. Sizing of the indentations detected is done in 2D and mirror-dependent field of view deteriorations are considered. These lead to local differences in the spatial discretization up to 10%. The smallest indentation size detectable is 50\(\mu m\) and possible smaller indentations are not considered in the post-processing.

![Table 6.2: Single particle defouling experiment: set-up variable ranges.](image)

![Table 6.3: Single particle defouling experiment: final HSC settings.](image)
6.3.2 Results

Examination of indentations

Examples of single particle indentations are presented in Fig. 6.6. The left hand display shows indentations of a PFTE coating made by POM particles used as reference material and the right-hand display shows such indentations from dry-ice particles upon the same fouling. The indentations from spherical POM particles are round but these from dry-ice particles are variously shaped.

Figure 6.6.: Microscopy images of indentations on PTFE from POM reference material particles (left) and dry-ice particles (right).

Furthermore, the dry-ice particles produce multiple indentations from single particle impacts and this can be attributed to the disintegration process of the impacting particles. The secondary particles from this primary particle breakup hit the target in secondary impacts. This finding is accounted for in the post-processing. Preliminary examination of dry-ice impacts led to the decision to add a maximum of 3 most significant indentations from one particle impact to the particular defouling information.

Energy dissipation

An additional experimental review of the concept to apply coefficients of restitution for various particles to account for dissipated energy proportions is presented in section C.2 in the Appendix. It reveals that the method is applicable to
collect the data desired. Based on this, the major experimental results for the
defouling energy are discussed in this section.

Figure 6.7 shows a set of typical results from dynamic indentation tests made
to assess the defouling energy. The left hand graph shows the coefficients of
restitution as a function of Stokes number for POM reference material particles
interacting with clean and PTFE fouled targets and the right-hand graph shows
the corresponding indentations and the resulting defouling function. Note that
the indentation diameters are shown as a function of Stokes number in this
case. This is valid because the particles used are uniform in size meaning that
the restitution functions and the defouling functions are comparable, which
is desired in the discussion below. The indentation size is normalized by the
maximum indentation size detected considering all datasets recorded.

Figure 6.7.: Experimental results for PTFE fouled targets and POM particles -
coefficients of restitution (left) for unfouled and fouled target and
corresponding defouling data (right).

Results comparable to the above PTFE/POM experiments are displayed in
Fig. 6.8 for stainless steel reference material particle indentations upon blades
coated with ORIG2 fouling. The PTFE impacts show most significant differences
in coefficients of restitution for low Stokes numbers (i.e. low impact velocities)
and this difference is not detectable for Stokes numbers higher than $St_B = 165$.
The impacts of stainless steel particles upon ORIG2 fouling show a different
restitution behaviour. A measurable difference of coefficients of restitution can
be detected in the range of Stokes numbers from $St_A = 320$ to $St_B = 1840$. 
Figure 6.8.: Experimental results for ORIG2 fouled targets and Stainless Steel particles - coefficients of restitution (left) for unfouled and fouled target and corresponding defouling function (right).

The comparability of the lower bound of the Stokes number range, which describes the onset of defouling erosion for ORIG2 fouling, is visible when comparing the defouling data to the corresponding restitution data. This lower range cannot be measured in the restitution data from POM particles upon PTFE coating because even the slowest particles investigated (i.e. 0.7 m/s impact velocity) caused a measurable indentation.

Defouling data

It is shown in section C.2 in the Appendix that the defouling diameter is linearly dependent on the impact particle diameter and that it is logarithmically dependent on the impact velocity. This finding is used in the presentation of typical defouling results and those are discussed below.

Figure 6.9 contains defouling data from dry-ice indentations upon PTFE fouled targets and the corresponding correlations. The left hand display shows these results for normal impacts (i.e. 0°) and the right-hand display such for angular impacts (i.e. 60°). A more significant scattering of the data is detected when comparing the results for dry-ice to those for reference material and this can be attributed to the disintegration and the irregular shape of dry-ice
Figure 6.9.: PFTE defouled with dry-ice - normal impact defouling (0°, left) and angular impact defouling (60°, right).

particles which may cause variously shaped and sized indentations and secondary particle impacts.

In general, a dependence of defouling on impact angle is negligible for PTFE. However, an increase in scattering is detected for the angular impacts in the range of impact velocities from 5 to 20 m/s. It is not accounted for this scattering in the actual model formulation and this may cause increasing uncertainties in the predictions of angular indentations.

Table 6.4 shows the key information describing the defouling functions derived from the experiments. The onset of erosion is described by the velocity values corresponding to the positions where the logarithmic correlations cross the abscissa. Comparable values are detected for reference material and dry-ice particles. The velocity values from reference material are displayed as equivalent dry-ice velocities and hence these are comparable.

In the second block of the table (i.e. Coeff. of Determination) the corresponding coefficients of determination of the defouling correlations are listed. A trend can be detected in most of the cases and it shows that the scattering of the defouling data increases if dry-ice particles are used compared to reference material data and if natural fouling is used compared to artificial fouling.

It must be noted that there was almost no defouling detectable for angular dry-ice impacts upon ORIG1 fouling, which explains the very low coefficient of
Table 6.4.: Overview of the key numbers describing the derived defouling functions for all parameters considered.

determination (i.e. $R^2 \approx 0.07$). The logarithmic correlation of this dataset is formally not valid but it is decided to accept this uncertainty here to be able to provide a comparable description for all materials considered.

The results for the whole range of materials and parameters investigated can be found in section C.3 in the Appendix and these show comparable features for all material pairings investigated. The results with the lowest coefficient of determination are achieved for ORIG1 fouling; this may be caused by the viscous nature of this particular fouling material compared to the others investigated.

**Correlated total results**

Correlated trends from the experimental data of all parameters investigated are shown in Fig. 6.10 and 6.11. The left hand display in Fig. 6.10 shows dissipation factors derived from comparison of correlated experimental restitution data with Eqn. (6.3) and (6.7) and the right-hand graph shows the corresponding defouling functions for reference material particles. As it is done above when discussing Fig. 6.7 and 6.8, the defouling functions are plotted against Stokes number for comparability.

The most significant proportions of energy are required to remove ORIG2 fouling in the range of Stokes numbers from 750 to 1250. A maximum dissipation factor of approximately 0.11 is detected for a corresponding dry-ice impact velocity of approximately 80 m/s with an 1.5 mm particle (i.e. Stokes number of 1000). Further significant proportions of energy are consumed for defouling of PTFE and SALT layers in the range of low Stokes numbers. Dissipation factors

<table>
<thead>
<tr>
<th>Particle, Angle</th>
<th>PTFE</th>
<th>SALT</th>
<th>ORIG1</th>
<th>ORIG2</th>
<th>PTFE</th>
<th>SALT</th>
<th>ORIG1</th>
<th>ORIG2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Onset of Erosion - $v_{crit}$ $[\text{m/s}]$</td>
<td>Coeff. of Determination - $R^2$ $[1]$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ref, 0°</td>
<td>0.44</td>
<td>2.33</td>
<td>17.28</td>
<td>13.14</td>
<td>0.90</td>
<td>0.77</td>
<td>0.50</td>
<td>0.85</td>
</tr>
<tr>
<td>dry-ice, 0°</td>
<td>1.15</td>
<td>2.75</td>
<td>20.97</td>
<td>10.38</td>
<td>0.74</td>
<td>0.64</td>
<td>0.50</td>
<td>0.42</td>
</tr>
<tr>
<td>dry-ice, 60°</td>
<td>2.20</td>
<td>7.12</td>
<td>20.09</td>
<td>14.01</td>
<td>0.72</td>
<td>0.73</td>
<td>0.07</td>
<td>0.52</td>
</tr>
</tbody>
</table>
lower than 0.10 are found for PTFE at Stokes numbers higher than 75 and for SALT at such higher than 270. These numbers indicate either low impact velocities or small particles.

Based on the above results it can be seen that the energy requirement for defouling is negligible in most cases. Although defouling energy is not further considered in the later simulations in this work, circumstances may arise where it needs to be included, and the above results permit this.

All defouling functions for dry-ice are shown in Fig. 6.11 and these encompass the indentations for all fouling materials investigated and perpendicular (i.e.

Figure 6.10.: Total results - impact dissipation factors for various fouling materials (left) and corresponding defouling functions (right) for reference material particles.

Figure 6.11.: Total results - defouling functions for dry-ice at normal (left) and angular (right) impact at all fouling materials.
0°) as well as angular (i.e. 60°) impacts. It can be seen that the PTFE correlations are almost independent of the impact angle. Salt layers are more easily removed with increasing impact angles, although the onset of erosion occurs at higher velocities compared to normal impact indentations. For increasing impact angle the defouling of ORIG2 layers decreases while there is almost no defouling detectable for ORIG1 layers.

The results presented and the assumptions discussed above are used to predict defouling processes in application simulations and the corresponding procedure is described in the following section 6.4.

### 6.4 Numerical model development

This section comprises the implementation of the above theoretical model into both a Matlab and an Ansys CFX procedure. The main results from these calculations with the Matlab model are discussed and a comparison study of defouling erosion predictions for various fouling materials is presented.

Furthermore, the defouling energy assessment is discussed based on typical computational results and its dependence on particle size and impact velocity for various fouling materials is highlighted. The original model is compared with the Ansys CFX implementation, which required some adaptations, and a verification study of both models is briefly described.

#### 6.4.1 Set-up

The main descriptive equations (6.1) to (6.9) and (C.1) to (C.7) are directly developed into a Matlab procedure and this is used to predict erosive defouling situations. The procedure balances the defouling impact process only and is assumed that particle breakup follows the erosion. It is necessary to specify the particle and fouling material and the material dependent statistical data, which is used in Eqn. (6.7) to (6.9). This data is stored in external files and therefore it is possible to make changes to this database without changing the code. Such
a situation may be considered if for example the experimental framework will be extended or if new material pairings should be implemented into the model.

The calculation procedure is shown in Fig. 6.12 and this scheme is comparable to what is reported in section 5.4.1 for the particle breakup model. The equations used are directly referenced in the scheme. If the particle impact velocity is higher than the critical value the erosion procedure starts and if not the procedure is aborted and all erosion values are set to 0. If erosion is indicated, the Stokes number dependent impact dissipation factor (#1) and the impact diameters are computed (#2). These diameters are calculated for particle and reference material and the values are used to estimate the particle energy dissipation (#3).

In step (#4) impact properties such as the defouled area, its elliptical eccentricity and the resulting geometry of the indentation are calculated. In the final step the data is returned to the outer loop of the code. Intermediate values for impact angles not considered in the basic experiment are interpolated or extrapolated and it is assumed that there is no defouling erosion if the particles hit the wall tangentially (i.e. 90° impact angle).

![Diagram](image_url)

**Figure 6.12.** Schematic of the computational defouling erosion procedure.
6.4.2 Results

Typical results are computed with the procedure described above and these are discussed in what follows. Defouled area predictions from single dry-ice particle impingements are plotted in Fig. 6.13 and the upper display shows normal indentations upon a PTFE fouled target in the range of impact velocities from 10 to 100 m/s. The lower display shows comparable results for an impact angle of 60°.

The particles considered have a diameter of 1.0 mm and the meshing of the target plate displayed is adaptive and dependent on the particle size. The mesh size is 5% of the particle diameter considered. The defouling areas increase with increasing impact velocity in both cases and the elliptical model, which is used to account for indentation shape and displacement (see section C.1 in Appendix), is visible when the positions and the shape of the lower predicted indentations are compared to these of the upper ones.

Comparable results are presented in Fig. 6.14 for normal impingements of dry-ice particles upon variously fouled targets. All fouling materials investigated are considered and the impact velocity ranges again from 10 to 100 m/s. These indentation diameters reported in Fig. 6.11 are reproduced by the computa-

![Figure 6.13](image-url)  

**Figure 6.13:** Typical results from defouling computations of dry-ice particles at normal (upper) and angular (lower) impact upon PTFE fouling showing relative size, shape and position of defouled area.
tions and the smallest indentation displayed is 10 % of the primary particle diameter. Most defouling at low impact velocities can be seen for PTFE and least defouling is found for the ORIG1 coating. If increasing the impact velocity PTFE defouling remains most but these defouled areas from the other coatings become comparable to each other.

![Diagram showing defouling computations of dry-ice particles at normal impact upon variously fouled targets showing relative size, shape and position of defouled area.](image)

**Figure 6.14.** Typical results from defouling computations of dry-ice particles at normal impact upon variously fouled targets showing relative size, shape and position of defouled area.

Typical outcomes from the energy assessment procedure are shown in Fig. 6.15 and 6.16 for dry-ice indentations in normal direction. Particles with various sizes are considered and these are computed impacting PTFE (Fig. 6.15) and ORIG2 fouling layers (Fig. 6.16). The left hand displays in both figures show the defouled area predicted as a function of impact velocity. It is normalized by the maximum defouled area detected in this study. The particle size plays a major role in the defouling process and the onset of erosion is determined by the critical velocity in both cases.
Figure 6.15.: Defouling computation for PTFE - area (left) and energy (right) as functions of normal impact velocity and particle size.

Comparing the right-hand graph to the left hand graph reveals that the onset of considerable defouling energy proportions can be determined by the critical velocity for PTFE. The particle size increases the maximum defouling energy proportion but it shrinks the range of velocities in which this amount of energy is considerable by means of the approach presented here. The upper bound of this range and its width are determined by the Stokes number and therefore it is variable with particle size.

Comparison of the PTFE data to this of ORIG2 fouling reveals smaller defouled areas for ORIG2 defouling and a different range of velocities for measurable proportions of defouling energy. Note the extended velocity range in Fig. 6.16 compared to Fig. 6.15. The onset of measurable defouling energy as well as

Figure 6.16.: Defouling computation for ORIG2 - area (left) and energy (right) as functions of normal impact velocity and particle size.
the end of this range is determined by the Stokes number. The trend discussed above which indicates more significant maximum energy proportions for bigger particles compared to a wider velocity range but smaller maximum energy proportions for smaller particles is confirmed for this fouling material.

Based on these results it is decided to neglect the defouling energy contributions in the final application case simulations because small particle sizes and high impact velocities are expected in most of the cases. However, this study can be extended to assess the influence of defouling energy to the overall energy balance and further quantities predicted by the model such as CO₂ gas concentration, gas phase temperature or particle velocities in application case situations. These quantities may be discussed as a function of particle impact velocities and particle sizes.

The Matlab code was tested and some typical results are presented and discussed above. The implementation of the model into Ansys CFX and some principal results from this are discussed in the next section 6.4.3 below.

### 6.4.3 Implementation into Ansys CFX

A direct transformation of the model into Ansys CFX is not possible, because Lagrangian particle routines in CFX, which may cause defouling erosion in the case of particle wall interaction, utilize the erosion rate density $ER$ as an output variable. It is computed as the amount of particle mass hitting a certain area of the wall in a certain period of time (i.e. its unit is $\frac{kg \cdot m^2}{s}$) and it is a continuous variable, because it is exclusively used to predict crystalline material erosion and this can be integrated over time. The model presented here, however, specifies erosion as a binary variable and returns the diameter of an equivalent circular indentation inside which the fouling is assumed to be completely removed.

The above erosion rate density is defined as follows in Ansys CFX

$$ER := E_{erm} \cdot \dot{n}_p \cdot m_p.$$  \hspace{1cm} (6.11)
and it uses the variables number rate $\dot{n}_p$ and particle mass $m_p$. These link the Lagrangian particle tracking with the actual erosion variable $E$ and the latter is determined by the erosion model used (index: $erm$) such as the incorporated turbomachinery-specific erosion models from FINNIE [56] and GRANT and TABAKOFF [66].

To satisfy this necessary CFX formulation with the new model presented here (index: $hda$), the erosion variable returned by the model is modified as follows

$$E_{hda} = \frac{d_{IMP}}{d_p} \rightarrow \frac{\frac{\pi}{2} \cdot d^2_{IMP}}{\dot{n}_p \cdot m_p}$$

and if it is used in the above Eqn. (6.11) the defouled area from a single particle impact can be assessed in $[m^2]$.

Furthermore, it is necessary to make this variable independent from the wall mesh size, which means that the erosion rate variable cannot be used as a binary value because this would either cause a massive grid dependence of the predicted solution in CFX or require very fine wall meshing. To overcome this issue, the erosion rate from the new model is related to the local nodal area values $A_{node}$ of the wall mesh

$$er_{hda} = \frac{ER_{hda}}{A_{node}} = \frac{\frac{\pi}{2} \cdot d^2_{IMP}}{A_{node}} = \frac{A_{IMP}}{A_{node}} \rightarrow [0...1] .$$

By means of this procedure it is possible to account for indentations from small single particles on coarse wall meshes. In this case an uncertainty must be accepted in the precise prediction of the position of the indentation. However, the amount of defouling can be precisely predicted. Multiple single impingements can be accumulated at single wall nodes of the mesh until the area of influence of this particular node is totally defouled. Once total defouling is reached at one node, no further defouling is allowed and the erosion rate density is capped to unity.

An example which highlights the difference between the binary and the cumulative formulation is shown in Fig. 6.17. It presents the run up of the
erosion model implementation in Ansys CFX. The figure shows a single dry-ice particle with a diameter of 1.0 mm impacting a PTFE fouled surface (here semi-transparent) with an approximate impact velocity of 13 m/s at an impact angle of 60°. The particle disintegrates into 5 secondary particles on impact and an area with a diameter of approximately 300 µm is defouled.

The result is computed and displayed on a coarse wall mesh with a mesh width of 5 mm. In the left-hand display the result is treated as binary and the node at which the particle hits the wall is totally defouled because defouling was indicated by the model. However, the actual defouling diameter predicted by the model is only approximately 6 % of the nodal diameter and therefore the result must be adapted to the coarse wall mesh to avoid this massive overprediction.

The right-hand result, which was computed with the above modified formulation, allows an accumulation of multiple particle impacts at one node and the predicted defouling diameter corresponds to the actually defouled 6 % of the nodal diameter. Multiple impacts on this node are necessary to defoul the whole nodal area and this procedure is finally used in the CFX implementation of the model.

Eventually, the shape and displacement of the predicted indentations can be assessed by the ellipse values returned by the new model. However, this displace-
ment and shape information is not accounted for in the Ansys CFX implementation and this is caused by several issues due to the processing of geometrical wall mesh locators in the Lagrangian particle solver in CFX. Therefore, only the defouled area can be predicted.

Before starting the final validation case and application case simulations, both model implementations are verified and this is reported in the next part of this section.

6.4.4 Verification study

A verification study of the Matlab model and of the corresponding Ansys CFX implementation is carried out and the computational results of all model variables used are compared to these directly calculated with the underpinning equations of the model. The parameters discussed in the framework of this verification study are listed in Tab. 6.5.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range tested</th>
</tr>
</thead>
<tbody>
<tr>
<td>Impact velocity</td>
<td>10, 100 m/s</td>
</tr>
<tr>
<td>Impact angle</td>
<td>0, 30, 60, 75, 90°</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>0.5, 1.0 mm</td>
</tr>
<tr>
<td>Fouling material</td>
<td>PTFE, ORIG1</td>
</tr>
<tr>
<td>Particle material</td>
<td>POM, dry-ice</td>
</tr>
</tbody>
</table>

*Table 6.5:* Parameters considered in the verification study for the new model.

This comparison study was straightforward because these basic model equations are used without further modifications or abstractions in both codes. All results investigated from both model versions show very good agreement of the particular variables tested and only minor rounding issues are detected. Special attention is paid to the interpolation and extrapolation procedures used to determine model variables between the impact angles of 0° and 60°, which represent the experimental nodes, and between 60° and 89.9°, which represents the maximum impact angle (i.e. almost tangential to the wall's surface).
Figure 6.18.: Typical results from verification study - defouling function (left) and energy dissipation (right); comparison between computed (NUM) and analytically obtained values (ALY).

There are no mistakes found and typical results from the verification study are shown in Fig. 6.18. The left-hand display shows the comparison between computed and analytically determined defouling diameters (here ALY) for both particle sizes considered and dry-ice particle impacts upon PTFE fouling. The right-hand display shows the same comparison for the predicted amounts of defouling energy. The most significant difference encountered between the numerical and the analytical values is 0.72 % in case of the defouling energy.

Based on the above results both model implementations are assumed to be verified and usable for the final studies. Both the particle breakup and the erosion model implementations in Ansys CFX are used in the next Chapter 7 to investigate a validation case experiment in the wind-tunnel. After this, both models are finally used for an application case simulation of typical defouling test carried out at the test-rig with a GE CF6-50 test-engine. This application case study is presented in Chapter 8 and it represents the final step of this project.

6.5 Summary of defouling erosion modelling

A new defouling erosion model has been presented and it is based on an extensive experimental database dealing with the defouling of variously fouled targets with various particle materials. The examination of this database revealed that
it is possible to use the particle’s coefficient of restitution as a function of the near-wall Stokes number to account for the amount of energy necessary for defouling in a certain range of impact parameters. Furthermore, it was shown that the amount of fouling removed (i.e. the indentation diameter) is a function of the impact particle size, of its velocity and of the impact angle.

The new model was used to compare various defouling scenarios with dry-ice particles and fouling materials typically used in aircraft compressor defouling experiments. Also, the defouling energy was discussed for some typical situations and it was decided to neglect this amount of energy in the overall energy balance which underpins the particle breakup model. However, it was shown that these amounts of energy are not negligible in all cases.

Finally the implementation of the model into Ansys CFX was described and both versions were verified against the statistical database underpinning the model. The maximum deviations encountered between computations and analytical solutions were as low as 0.72 % and can be attributed to slight differences in rounding procedures and overall accuracy. The Ansys CFX implementation of the new defouling erosion model is used in the validation and in the application case simulations presented in Chapters 7 and 8.