Chapter 11 Experimental Study and Modelling of Particle Behaviour in a Multi-stage Zigzag Air Classifier



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Abstract In most industrial solid processing operations, the classification of particles is important and designed based on the terminal settling velocity as the main control parameter. This settling velocity is dependent on characteristic particle properties like size, density, and shape. Turbulent particle diffusion is the other key property controlling the efficiency of the separation. In this project, multi-stage separation experiments of a variety of materials have been performed using different flow velocities, mass loadings of the air, number of stages. Separation has been investigated separately concerning particle size, particle density, and particle shape. Continuous operation in terms of solid material and airflow has been mostly considered. However, variations in mass loading and pulsating operation of the fan have been investigated as well. The performance has been analyzed and discussed with respect to the separation functions, for instance regarding separation sharpness. Several modelling approaches have been checked and/or developed to describe theoretically the corresponding observations. After fitting the free model parameters, a very good agreement has been obtained compared to experimental measurements. Finally, the reduced model has been implemented into the central software DYSSOL.

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1 Introduction

The treatment of raw materials, intermediates, products, and waste is one of the most important processes for many industrial applications. Usually, the final process outcome depends strongly on the quality of separation. Separation by particle size is mostly done by sieving. For lower cut points (for a particle diameter in the order of mm), air classifying performs better because fine particles often adhere to and block the openings of the sieves. One apparatus for air classifying is the zigzag air classifier. This system has been known for a long time [1-3]. It is widely used for a variety of industrial applications, e.g. for classifying shredded PET bottles [4], municipal solid waste [5], scrap cables, or stalks and leaves for the tea and tobacco industry [6].

The main advantage of multi-stage air classifying is the wide range of possible cut sizes, in the range of micrometers to several millimeters. Sorting (separation by density) can be done within a wide density range as well. Separation is done based on the differences in settling velocity, which is the main characteristic parameter and is determined by particle properties as size, density, and shape [6].

Obviously, the air velocity in any separation chamber impacts the particle dynamics, in particular with respect to the flow direction. Due to this fact, the zigzag air classifier has a wide field of possible applications. The mass flux of one stage in practical applications is typically between 5 and 15 t/(m h); an even higher throughput can be reached by using several channels in parallel. The number of stages affects the separation performance since, at every stage, separation of fine and coarse (or light and heavy) particles occurs as the particles flow across the air stream. Therefore, every particle that leaves the channel has been separated repeatedly, which leads to a high operational efficiency. Additionally, the process can be linked to pneumatic conveying without the requirements for any additional device [6].

However, problems are also encountered when using a zigzag air classifier (ZAC). In particular, variations in properties of the feed (in size, density, or shape) e.g. due to segregation in the silo, eventually lead to local and temporal fluctuations of the mass loading of air. This affects the efficiency of the separation in a negative way. Due to these fluctuations, pulsations of the air stream may also be observed. All in all, the unknown dynamics of the process lead to insufficient reliability of the ZAC operation, reducing separation efficiency. Though the efficiency might be increased again by employing a larger number of stages, those cause additional pressure loss, increasing energy consumption. As a consequence of this trade-off, it is expected that an optimal number of separation stages exists for a given process.

Since ZACs have been used for many decades, they have been the topic of several investigations. Selected publications are discussed in what follows. For instance, Worrell and Vesilind [7] investigated the separation performance of different air classifiers based on various throat configurations. They used municipal solid waste to separate light (paper and plastics) and heavy (aluminum and steel) materials and introduced a new concept to evaluate the operational efficiency. The total efficiency was defined as the product of the fractional recoveries of light and heavy material in the overflow and underflow. Therefore, the highest efficiency of 100% can only be

reached if 100% of the lightweight material is discharged as light product and 100% of the heavyweight material is delivered as heavy product.

The operational efficiency of ZACs at low particle concentrations has been investigated by Senden [5] who used square pieces of paper and porous polystyrene spheres as test materials during the experiments. He analyzed the influence of different channel depths and bending angles (90°, 120°, 150°) and found the 150° case showing the highest separation efficiency associated with an enormous increase of particle residence time. Furthermore, he developed a stochastic model to describe the separation behavior based on observations of every single stage. Rosenbrand [8] extended Senden's model [5] for high particle concentrations using a dimensionless correlation.

Vesilind and Henrikson [9] studied the influence of feed rate on the separation performance in a zigzag channel with a bending angle of 120° using square-shaped plastic and aluminum pieces. It was shown that particle residence times decrease with increasing feed rate; the same applies to separation efficiency. Both effects were ascribed to an increased particle-particle collision frequency.

For performance comparison of different air classifiers, Biddulph and Connor [10] developed a simple test based on the estimation of effective diffusivity; good separation efficiencies were assumed to be connected with low diffusivities.

The research group around Tomas [11, 12] developed a model to describe the separation performance in a ZAC. This model agreed well with experimental data measured by separation experiments of glass beads, sand, split, and gravel at low mass loadings of the air. One important advantage of their model is a flexible application concerning separation by size, density, or shape. The zigzag air classifier was found to deliver satisfactory to good separations, and this at low energy consumption.

The separation of PET flakes by particle shape in a zigzag separator has been studied in several studies [4, 13, 14]. Using a low mass loading of the air, the process showed good separation efficiency.

Several investigations can also be found in the literature (e.g., [13, 15]) concerning the simulation of one- and multi-phase flows in zigzag-shaped channels using Computational Fluid Dynamics (CFD). However, only few of these publications attempted to quantify separation performance.

The aim of the present investigation was to investigate in a systematic manner the processes leading to particle separation in a ZAC, by combining in a suitable manner theoretical, experimental and numerical investigations.

The installation used for all studies is shown in Fig. 1. The pilot-scale air separator used in this research consists of the zigzag channel featuring four exchangeable channel modules aligned vertically and housing two segments each, which are connected under a prescribed inclination angle. A controllable blower drives the air in a closed circuit through the apparatus. Air flows through the inflow pipe and then from bottom to top through the zigzag channel, through an aero-cyclone and a filter before it re-enters the blower. Particles are fed to the system through a small square duct at mid-height of the zigzag channel by means of a controllable vibration conveyer connected to a hopper. The separated material is collected in two containers, one for



Fig. 1 Principle sketch of the investigated pilot-scale zigzag air classifier with (1) aero-cyclone, (2) zigzag channel, (3) container for fine fraction, (4) container for coarse fraction, (5) hopper, (6) screw feeder, (7) filter, (8) inflow pipe, (9) fan

the coarse fraction falling down into the underflow bin, and one for the fine fraction lifted with and separated from the airstream by a cyclone into the fine fraction bin.

Many different process conditions have been considered and analyzed in a systematic manner using this system. Thanks to such extensive studies, it should become ultimately possible to derive best-practice recommendations for designing and using a ZAC in an optimal manner for a given process. Since all the results of this project have been already extensively published, the rest of this chapter consists mainly in summarizing the most important findings regarding each aspect of this combined study.

2 Research Strategy

Considering the complexity of the process, a combination of theoretical, numerical and experimental studies was considered best to get a deep insight regarding the controlling physical mechanisms, with a view toward optimal design and operating conditions. The corresponding subprojects are described in Fig. 2 and correspond to following steps:

- Theoretical description of a single spherical particle settling in a gas flow under laminar or turbulent conditions;
- Experimental investigation of fluid velocities, turbulent properties and vortex structures in the ZAC;
- Numerical simulations of fluid velocities, turbulent properties and vortex structures in the ZAC;
- Experimental investigation of particle trajectories in the ZAC;
- Numerical simulation of particle trajectories in the ZAC (coupling Computational Fluid Dynamics with either Discrete Particle Model—DPM—or Discrete Element Model—DEM);
- Experimental investigations of separation based on particle size, particle density, particle shape;
- Derivation of a simplified model of particle separation in the ZAC and integration of this model into the central simulation platform DYSSOL developed in the group of S. Heinrich at the Technical University Hamburg.



Fig. 2 Research strategy used for this project

Name	Equation
Equation of motion	$\frac{\mathrm{d} \mathrm{v}}{\mathrm{d} \mathrm{t}} = \frac{1}{\mathrm{t}_{\mathrm{R}} \mathrm{v}_{\mathrm{s}}} \left(\mathrm{v}_{\mathrm{s}}^2 - \mathrm{v}^2 \right)$
Relaxation time t _R	$t_{R} = \left(\rho_{p} + j \rho_{f}\right) \sqrt{\frac{3d_{p}}{\rho_{f}(\rho_{p} - \rho_{f})g}}$
Relaxation distance s _R	$s_{R} = t_{R}v_{s} = \frac{3d_{p}(\rho_{p}+j\rho_{f})}{\rho_{f}}$
Velocity-time law	$v = v_{s} \frac{(v_{s}+v_{0}) \exp\left(\frac{2}{t_{R}}(t-t_{0})\right) - v_{s}+v_{0}}{(v_{s}+v_{0}) \exp\left(\frac{2}{t_{R}}(t-t_{0})\right) + v_{s}-v_{0}}$
Velocity-distance law	$v = \sqrt{v_s^2 - (v_s^2 - v_0^2) \exp\left(-\frac{2}{t_R v_s}(s - s_0)\right)}$
Distance-time law	$s = s_0 + v_s \left(-(t - t_0) + t_R \ln \frac{(v_s + v_0) \exp(\frac{2}{t_R}(t - t_0)) + v_s - v_0}{2v_s} \right)$

 Table 1
 Analytical solution for a turbulent flow around a settling particle in the Newton regime

3 Main Results

3.1 Theoretical Study

The settling process of particles in the Stokes and the Newton regimes are of central importance for understanding separation in the ZAC. Considering only spherical and isolated particles, it is possible to obtain full analytic solutions for this configuration, in particular regarding terminal settling velocity and corresponding relaxation times. The main results of the theoretical investigations carried out during this project have been documented in [16]. Additional details and information can be found (in German) in [17]. For instance, the main resulting equations regarding the behavior when a turbulent flow is found around the particle are given in Table 1, in which the notations of [16] have been kept.

Using these relations, it is now easily possible to derive corresponding results for relevant materials considered in the rest of this study. For instance, the behavior of gravel settling in air is shown in Fig. 3.

3.2 Experimental Investigations Regarding the Turbulent Air Flow

Apart from systematic separation experiments described later in this chapter, the physical processes controlling the coupled behavior of turbulent flow and particles have been investigated in detail. For this purpose, a variety of measurement methods have been used. The simplest ones relied on probes placed within the set-up. In this



manner, it was for instance possible to investigate the pressure drop induced by the channel (Fig. 4).

The results of the measurement campaigns have been used for two different purposes:

- Foster our understanding of the processes controlling particle separation;
- Support accompanying numerical simulations, by delivering boundary conditions and reference data for validation.

Regarding the latter point, laser-based measurement techniques have been used. Being purely optical and thus non-intrusive, they have the advantage of not perturbing the observed process in any manner. In a first step, Laser-Doppler Velocimetry (LDV) has been employed in the entry section of the zigzag channel (Fig. 5). In this manner, proper inflow boundary conditions have been obtained for mean velocity and







turbulence intensity. Those form the basis for all simulations relying on the Unsteady Navier-Stokes Reynolds-Averaged (URANS) equations, discussed in the next subsection. Using this experimental information as boundary conditions, it becomes possible to compute only the zigzag channel itself, excluding the fan section and the coarse fraction (i.e., bottom) container from all further simulations. Since the employed installation is large, this is important to limit the volume of the simulation domain and, therefore, the necessary number of discretisation cells, allowing a better resolution and/or shorter computational times.

In a second step, the focus has been mainly set on Particle Image Velocimetry (PIV). Note that such PIV measurements are very challenging in our pilot-scale apparatus, since many difficulties must be met: large-scale system, leading to measurements several meters above ground level; related safety issues (laser protection); very complex geometry; limited optical access (a large part of the channel had to be reconstructed out of high-quality acrylic glass to enable laser-based measurements); very dusty environment; strong vibrations. Most PIV studies documented in the scientific literature investigate academic configurations under well-controlled conditions, very often in a dedicated optical laboratory. In the present case, PIV measurements must take place in a very large experimental hall hosting more than 10 different experiments—sometimes running simultaneously.

The employed PIV setup is shown in Fig. 6. The acquisition of images at 5 Hz was carried out for a variety of process conditions.

By analyzing the obtained PIV images, a variety of information can be obtained. Both instantaneous and average velocity fields have been derived, as shown in Fig. 7. Additionally, the dominating features of the vortical structures found in the channel have been identified. Finally, information is also obtained regarding turbulence intensity and the main frequencies of the fluctuations observed in the channel. This first investigation is helpful to identify key features of the complex and highly unsteady turbulent air flow within the zigzag channel.



Fig. 6 View of the PIV hardware around the zigzag channel (left). Zoom on the PIV camera imaging the calibration target within the channel (centre). Laser light-sheet used for PIV (right)



Fig. 7 Exemplary PIV images within the zigzag channel: instantaneous (left) and average flow field with recirculation zone (right) at the same location

3.3 Numerical Investigations Regarding the Turbulent Air Flow

In parallel to these first experimental investigations, a large number of numerical simulations based on Computational Fluid Dynamics (CFD) have been carried out, first considering only the gas flow. For all these simulations, the exact geometry of the installation has been taken into account and used as a basis for discretisation. First simulations considered the whole system starting at fan outlet. This leads unfortunately to a very large gas volume; for this reason, a satisfactory resolution could not be achieved with reasonable computing times. In order to solve this issue, the LDV measurements described previously have then been used systematically as boundary conditions. In this manner, only the zigzag channel itself needs to be taken into account in the numerical simulation, reducing drastically computational times.



Fig. 8 Instantaneous velocity field obtained by URANS simulations in one segment of the ZAC under identical conditions and resolution for different turbulence models: standard k- ϵ (left), k- ω -SST (center), and SAS (right)

The flow in the zigzag channel is highly turbulent. Considering the complexity of the geometry and of the resulting flow features, high-fidelity simulations like direct numerical simulation (DNS) or large-eddy simulation (LES) would be recommended. However, DNS is simply impossible for this configuration; a single LES simulation would be acceptable, but systematic studies involving additionally particles are again beyond reach. The only approach allowing many different simulations relies on the unsteady RANS equations. As a consequence, in a second step, the impact of the turbulence model used in all further URANS simulations has been assessed. During the course of this 6-year research project, URANS simulations have been carried out using different versions of the industrial software ANSYS-Fluent, STAR-CCM+, or OpenFOAM, depending on license availability and on the proposed models. As a matter of fact, no relevant difference has been obtained among these different software solutions when using similar resolution and models. On the other hand, the impact of the employed turbulence model was found to be extremely high. As an illustration, Fig. 8 shows instantaneous results obtained in the same segment of the channel with the same grid resolution and at the same time with three different, well established turbulence models: standard k- ε , k- ω -SST (Shear Stress Transport), and SAS (Scale-Adaptive Simulation).

These turbulent flow simulations revealed that the standard k- ε model does not lead to sustained unsteady features; after computing about 1 s of physical time, a steady solution without any fluctuation is established within the channel, which is in contradiction to the experimental observations. Using now the k- ω -SST model, only very weak periodic fluctuations involving a single large-scale vortex pair are observed in the corner of the channel; again, this behavior does not coincide with experimental measurements. Only the SAS model is able to deliver a highly unsteady velocity field involving a number of small-scale vortices, in qualitative agreement with experimental observations. Unfortunately, the SAS model (or equivalent formulations) are not available in all simulation platforms yet; additionally, these models come in general with a noticeably higher computing time, since finer grids and smaller timesteps are required to get properly resolved features. Further studies will be necessary before getting final statements regarding the recommended URANS turbulence model for the ZAC.

3.4 Experimental Investigations Regarding the Particles

After having properly characterized the turbulent air flow, further experimental investigations elucidated the behavior of the particles during the separation process in the ZAC. In order to avoid any perturbation of the system, optical measurements have been again preferred, this time relying on shadowgraphy. This means that a background illumination is employed, and the shadows of the particles on the camera image are post-processed to get a variety of information, like particle number density, particle movement, particle velocity (using consecutive images), and possibly particle shape and orientation. The main findings of these measurements have been documented extensively in [18]. Apart from delivering useful information regarding the local particle velocity at different levels within the zigzag channel, this investigation also revealed the main characteristic particle movements, as shown in Fig. 9.

In particular, the following conclusions can be drawn from these measurements: the dominating motion for particles flowing downward is a sliding motion along the bottom wall of the channel; the flow separation found behind each channel bend is of central importance to explain particle trajectories, increasingly so for higher flow-rates; collisions of particles with other particles or with the channel walls play a prominent role to understand the non-homogeneous distribution of particle number density; the upward movement of the particles is dominated mainly by the features of the air flow and is more complex than the downward movement. These observations are essential to develop proper theoretical models able to describe particle separation with sufficient accuracy.



Fig. 9 Dominating particle trajectories identified by shadowgraphy along each bend of the zigzag channel

3.5 Coupled Simulations of the Particulate Flow Within the Zigzag Channel

Again, in parallel to the experimental study discussed previously, a variety of numerical simulations have been carried out in an effort to describe the behavior of the particles within the turbulent air flow found within the zigzag channel. Keeping in mind, as discussed previously in Sect. 3.3, that it was already extremely challenging to solve for the turbulent air flow *without* any particles, it is clear that this objective is extremely ambitious, both regarding the needed computational resources (computing time and memory) as well as model accuracy (availability of sufficiently accurate numerical models).

The first attempt in the project was to couple the URANS simulation with a very simple particle model (Discrete Particle Model, or DPM) using a one-way approach, considering all particles as points, neglecting any influence of the particles on the flow, and disregarding all collisions. These very strong simplifying hypotheses are helpful to reduce computational times; however, it is clear from the start that getting suitable predictions with such simplifications would be a good surprise. Indeed, and independently from the employed turbulence model, it has been fully impossible to get any acceptable agreement regarding process outcome using such simplifications, as exemplified in Fig. 10. At best, some qualitative trends can perhaps be derived from such simple simulations; but quantitative predictions appear to be impossible. More details regarding such comparisons with separation experiments discussed in the next subsection can be found in [14].

In an effort to improve the accuracy of the numerical predictions, it was decided to switch from the simple DPM model to the more advanced DEM approach (Discrete Element Model). In principle, URANS-DEM simulations come at a considerably higher numerical cost but open the door for truly coupled simulations between turbulent flow and particles, and are able to directly take particle collisions into



account. Therefore, it is expected that such numerical predictions should be closer to the experimental observations. However, depending on the employed software, such simulations do show also some limitations. Since open-source solutions are of course advantageous for fundamental research projects, it was decided to perform these URANS-DEM simulations using the coupled open-source software CFDEMcoupling [19]. CFDEMcoupling combines the C++-based open-source software environments OpenFOAM (for CFD) and LIGGGHTS (for DEM). Hence, CFD and DEM calculations rely on two separate codes. The interaction between the two calculations is realized by exchanging relevant information with a predefined timestep. Unfortunately, advanced turbulence models like SAS are not available in CFDEMcoupling. Looking back at the results of Sect. 3.3, the "best" model currently implemented there is the k- ω -SST model. Even if our previous study has demonstrated that this model leads only to weak flow fluctuations involving few large-scale vortices (at the difference of experimental observations), it had to be kept for the present simulations. In Fig. 11, the numerical prediction for classification based on particle density is shown, in comparison with experimental data.

In particular, this study revealed an unexpectedly strong influence of the employed drag model. For Fig. 11, the model of Di Felice [20] has been retained. Switching to another model, or modifying the poorly-known coefficients appearing in the drag law, the results become very noticeably different. Using model fitting, it is then possible to reach in principle a good agreement by comparison with the separation experiments discussed in the next subsection. However, this is obviously not a satisfactory solution. This highlights the need for further research regarding CFD-DEM simulations and all underlying models in the future.



Fig. 11 Separation function predicted by URANS-DEM using the drag model of Di Felice in comparison with own experimental results when separating particles based on their density

3.6 Separation Experiments

During the course of this project, uncountable separation experiments have been carried out. It is not the purpose of this section to discuss all corresponding results. Interested readers can find more information in the references listed at the end of this work, in particular in [21]. Further publications on this topic are currently under review or being written.

In order to get insight of practical relevance, different kinds of separation experiments have been documented, in chronological order:

- Separation based on particle size, for a variety of materials (constant air flow);
- Separation based on particle density (constant air flow);
- Separation using a pulsating air flow;
- Separation based on particle shape (constant air flow).

The experiments corresponding to the two last steps are currently being postprocessed, and are thus left for future publications. Separation of sand and gravel based on particle diameters has been documented in [21]. The results are exemplified in Fig. 12 for gravel, with particle diameters between 0.1 and 9 mm and a high sphericity of 0.85, all particles having the same density.

Concerning now density-based separation, the central objective was to investigate this effect on its own. As a consequence, the diameter and shape of the particles should be kept identical. Additionally, since optical measurement techniques should be used, it was desirable to directly encode the particle density in the acquired images. After a long search, it was finally possible to find suitable particles of different color (see



Fig. 12 Measured total efficiency for the separation of gravel as a function of mass loading (left) or channel flow velocity (right)



Fig. 13 Spherical particles used for density-based separation experiments. Each color corresponds to a different density, with identical diameter. In this picture, the image post-processing software developed for an automatic recognition of the particles in the coarse-fraction container has been validated by comparison with a manual treatment. Circles correspond to individual particle detections, circled numbers to particle groups

also Fig. 13), all spherical, with the same diameter and density, at a still acceptable price, and hence perfectly suitable for corresponding experiments.

4 Development of Reduced Models

All these results have been used to check, validate, and improve models able to describe particle separation in the ZAC. Of particular importance for this purpose are:

- The reference data for comparison provided by the separation experiments (for instance Fig. 12);
- The identification and quantification of typical flow features, necessary to drive model development (for instance Fig. 7);
- The identification of relevant particle movements (for instance Fig. 9), shown again in an exemplary manner in Fig. 14;
- The theoretical investigations given for a single particle at the beginning of this chapter, together with our knowledge regarding the importance of turbulent particle diffusion.

Combining all these features, and based on the existing literature regarding ZAC modelling, different approaches can be developed, either building directly on top of existing models [11, 22], or by proposing new directions.



Fig. 14 Typical particle movement controlling the classification process

4.1 One-Dimensional Discretized Approach

One original approach regarding the modelling of the process is the one-dimensional discretisation of the separation process in axial direction, as described schematically in Fig. 15. This approach has been presented in detail in the PhD Thesis of Hannes



Fig. 15 Balance of particle fluxes around a discretized portion of the zigzag channel at position z

Mann, "Experimentelle Untersuchung, Modellierung und dynamische Simulation der mehrstufigen turbulenten Partikel-Querstromklassierung" (Otto-von-Guericke-Univ. Magdeburg, 2016). In principle, it amounts to a discretisation of the zigzag channel in a (possibly large) number of compartments exchanging mass fluxes of particles with specific properties through their boundaries. Using an iterative approach, steady-state conditions can be reached.

Unsteady predictions are in principle possible as well. Though this model is attractive and could deliver a high accuracy, it requires a good knowledge of many parameters and is not well suited for an integration into the central simulation software DYSSOL. For this reason, alternatives are needed.

4.2 Improving Classical Models

During the course of this investigation, two established models have been revisited. Of particular importance is the turbulent particle diffusion, being a central control parameter regarding separation efficiency. Using the model of [11] while properly fitting the unknown model parameters, a very good agreement can be obtained for density-based separation, as illustrated in Fig. 16. However, one issue encountered in this modelling approach, is that the proposed range for turbulent particle diffusion is in complete disagreement with the experimental observations gained during this project. It was thus decided to revisit the original model of [22] in the light of the new experimental findings. This important part of the project is the subject of a publication currently under review, and will not be described further here in the interest of space.





As exemplified in Fig. 17, it leads to an excellent agreement with the measurement data.

4.3 Implementation in DYSSOL

The final step of this project is an implementation of the reduced models into the central software DYSSOL, derived at the Technical University Hamburg in the group of S. Heinrich. This has already been carried out for the model derived from [11], as illustrated in Fig. 18. In this manner, coupled simulations involving zigzag classifiers can readily be carried out in this context.



Fig. 18 Screenshot from DYSSOL (left: computation results; right: employed setting) showing the implementation of the ZAC model derived from the model of Tomas and Gröger [11]

5 Conclusion and Perspectives

The zigzag air classifier is a device of high practical importance for a variety of industrial applications. Additionally, the processes controlling separation in the zigzag channel are extremely interesting from a fundamental point of view, since they highlight the importance of coupled aspects (modification of the turbulent flow induced by the particles; particle-particle and particle-wall collisions; particle swarm effects...). In this combined study, theoretical developments, systematic experiments, and numerical simulations relying on different approaches have been combined to elucidate the controlling parameters and to develop reduced models, suitable for integration into simulation platforms like DYSSOL. It appears that, after proper model fitting, a good agreement can be obtained between measurement data and model predictions. Nevertheless, the large differences still found between experiments and simulations reveal the need for further studies before fully predictive numerical studies of practical systems become possible with standard computational resources.

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