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CFD METHODS AS A MODERN TOOL IN OPTIMISATION OF HYDRODYNAMIC CONDITIONS IN MAGMA CRYSTALLIZERS

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Abstract: Selected parameters concerning the optimisation of hydrodynamics in magma crystallizers are discussed. At this stage, results of CDF (Computational Fluid Dynamics) simulations are shown, focused on the effect of the geometrical configuration of a crystallizer on energy dissipation rate, axial velocity field and general hydraulic efficiency.

The influence of the shape of the apparatus' bottom, diameter of the stirrer, its location and presence of the draft tube on, respectively: (i) unit power input distribution, (ii) the average mixing power, and (iii) pumping capacity have been taken into consideration.

The results obtained from simulations have been compared with experiments and literature data.

Keywords: CDF, crystallization, hydraulic efficiency

Notation

Symbols

- d impeller or draft tube diameter [m],
- D vessel diameter [m],
- g acceleration due to gravity [m/s²],
- h height [m],
- P power mixing [W],
- s number of revolutions [1/s],
- V volume [m³],
- Vp pumping capacity $[m^3/s]$,
- ε unit power input [W/kg],
- ρ density [kg/m³],
- η viscosity [Pas],
- $Fr = s^2 d_m/g$ the Froude number for the mixing process,

$$\begin{split} &\operatorname{Re}=sd_m^2\rho/\eta-\operatorname{the} \operatorname{Reynolds} \operatorname{number} \operatorname{for} \operatorname{the} \operatorname{mixing} \operatorname{process},\\ &\operatorname{Kp}=Vp/(sd_m^3)-\operatorname{the} \operatorname{volumetric} \operatorname{flow} \operatorname{number},\\ &\operatorname{Ne}=P/(\rho s^3 d_m^5)-\operatorname{the} \operatorname{power} \operatorname{number}.\\ &\operatorname{Indices}\\ &\operatorname{c}-\operatorname{liquid},\\ &\operatorname{m-stirrer},\\ &\operatorname{r}-\operatorname{draft} \operatorname{tube},\\ &\operatorname{max}-\operatorname{maximum}, \end{split}$$

1. Introduction

In the presented work, the influence of crystallizers' geometrical configuration on hydraulic conditions is analysed using the CDF technique.

This problem is particularly essential in the optimisation of crystallizers' shape in general, as well as in crystallization processes with chemical reactions or led by means of salting out, as especial cases. Recognition of the relationship between the geometry of the apparatus and turbulence distribution, *i.e.* zones of high micromixing, with regard to the reagents' physical and chemical proprieties, allows one to conduct the process more consciously thus improving homogeneity of the product and increasing average sediment size in the crystalline pulp.

In this article, the influence of the shape of the crystallizer's bottom, the location of the draft tube or stirrer in the vessel and their diameters on turbulence distribution, axial velocity field, mixing power and hydraulic efficiency is presented.

2. Range and results of the simulation

The calculations were carried out using the CDF (MIXSIM and FLUENT) packet for homogeneous liquids under the conditions of turbulent flow in the stable range of mixer work [1], *i.e.* in range of values of the Froude number above 1.6.

A cross-section of the investigated crystallizer is presented in Figure 1. A 3D grid example is shown in Figure 2.

In simulations and experiments the following parameters were considered:

- diameter of the stirrer or draft tube, expressed as a $d_r(d_m)/D$ relation, in the range of 0.37–0.55,
- two kinds of bottoms: flat and elliptic,
- position of the stirrer or draft tube, as a $h_{\rm m}/d_m$ relation, in the range of 0.17–0.40.

The liquid flow was directed down into the draft tube.

A three-blade axial flow impeller, of the LIGHTNIN A310 type, as in the MIXSIM library, has forced the movement of a medium.

In Figure 3, examples of energy dissipation rate in the crystallizer are presented, with and without the draft tube.

The difference between the maximum and average values of unit power input (Figure 3) is remarkable. In a system without the draft tube and with a flat bottom, the value of the maximum unit power input is about 28 times higher than the average value, and 33 times in a system with an elliptic bottom. When a draft tube is

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ave - mean.

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Figure 1. The investigated crystallizer



Figure 2. 3D grid in apparatus with elliptic bottom

used, these values are 15 and 28, respectively. The region of ε_{max} is always close to the working stirrer zone, which confirms the earlier experimental investigations of Laufhütte, Villermaux and Franke. Laufhütte [2] qualified the maximum value of $\varepsilon_{\text{max}}/\varepsilon_{\text{ave}}$ relation on 10, and Villermaux [3] on 2.4. In both cases, no draft tube was applied.



Figure 3. Local energy dissipation rate in various geometrical configurations

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Figure 4. Effect of the draft tube gap from the bottom on $\varepsilon_{\rm max}/\varepsilon_{\rm ave}$



Figure 5. The axial velocity distribution in the mixer with draft tube and flat or elliptic bottom

Franke [4] marked this value on 5, in the presence of a draft tube in the vessel. We should stress considerable differences between values from the literature and these obtained in calculations. However, in any case the presence of a draft tube reduced the difference between maximum and average values of unit power input. The values obtained from our simulations are higher by 3 to 5 than the experimental data. At this stage, it has not been possible to determine which of values are more reliable. It is yet possible to suppose that the levelling of the maximum value of unit power input due to the presence of a draft tube will contribute to the limitation of micro-mixing

zones. The reduction of micro-mixing zones, in the case of weakly soluble components and a shallow metastable zone, could enable one to reduce the intensity of primary nucleation.

No influence of the draft tube's location on $\varepsilon_{\text{max}}/\varepsilon_{\text{ave}}$ simply value has been observed (see Figure 4).

The geometry of a crystallizer strongly affects local values of axial liquid velocity (see Figure 5). When applying an elliptic bottom instead of a flat one, the axial flow is more uniform, particularly inside the draft tube, and the absolute maximum values are about 13% higher.

Computed values of the power number, Ne, for particular configurations, show a strong relationship with the geometry of the apparatus. The diameter of the stirrer (draft tube) seems to have particularly great influence (see Figure 6). In each of the analysed cases, an increase in the stirrer's diameter caused a decrease in the value of the power number, Ne. Results of experiments in the use of axial flow stirrers, without a draft tube, reported by Fasano [5] and Fořt [6] (Figure 6), confirm this tendency.



Figure 6. Effect of the d_m/D ratio on the power number, Ne, in the system: \blacktriangle CDF, and \bigtriangleup experiment – with a draft tube and flat bottom; \blacklozenge CDF, and \diamondsuit experiment – with a draft tube and flat bottom; \blacklozenge CDF, elliptic bottom; \checkmark Fasano [5]; + Fořt [6]

A very strong correlation between $d_{\rm m}(d_{\rm r})/D$, and the general hydraulic efficiency of crystallizer, determined as Kp/Ne, has also been confirmed for systems with and without a draft tube (see Figure 7). The determined values of Kp/Ne simplex have been almost 2.5 times higher for the mixer with a draft tube.

The literature data [5, 6] do not confirm such strong correlations. According to these authors, increasing the stirrer diameter caused only a moderate increase in the Kp/Ne value.

Our simulations are consistent with Chudacek's [7] experimental results. In both cases, the effect of the impeller's distance from the bottom on the power number, Ne, is the same. Chudacek studied power characteristics and flow rate in an apparatus with a draft tube and an A310 impeller.

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Figure 7. Dependence between hydraulic efficiency, Kp/Ne, and the diameter of the impeller, d_m , in a crystallizer: (a) with a draft tube, (b) without a draft tube; \blacklozenge flat bottom; \blacksquare elliptic bottom



Figure 8. Power number, Ne, versus distance from the apparatus' bottom, $h_{\rm m}$, for a system with: \blacktriangle CDF, and \vartriangle experiment – with a draft tube and flat bottom; \blacklozenge CDF, and \diamondsuit experiment – with a draft tube and elliptic bottom; \blacklozenge CDF, flat bottom; \blacksquare CDF, elliptic bottom; \times Chudacek [7]

However, we have observed that in a system without a draft tube the influence of the $h_{\rm m}$ value on the power number is much stronger (see Figure 8). Our numerical calculations show significant influence of the stirrer's distance from the vessel's bottom, expressed as $h_{\rm r}(h_{\rm m})/d_{\rm r}(d_{\rm m})$, on the value of hydraulic efficiency, Kp/Ne (see Figure 9). In the presence of a draft tube, an increase in the $h_{\rm r}/d_{\rm r}$ ratio causes an increase of the Kp/Ne value. A similar character of Kp/Ne dependence on $f(h_{\rm m}/d_{\rm m})$ has been seen in CDF simulations in the absence of a draft tube.

3. Conclusions

The obtained results have proven the existence of a strong relationship between the geometrical configuration of a crystallizer and power input dissipation and hydraulic efficiency, as factors influencing the optimisation of an apparatus, e.g. \oplus



Figure 9. Effect of stirrer distance from the apparatus' bottom $h_{\rm m}$ on hydraulic efficiency, Kp/Ne, in the vessel: (a) with a draft tube, (b) without a draft tube; \blacklozenge CDF, and \diamondsuit experiment – flat bottom; \blacksquare CDF, and \square experiment – elliptic bottom

under the conditions of (i) minimum power input and maximum pumping capacity, or (ii) minimal difference between ε_{max} and ε_{ave} .

Standard mixers applied in crystallization processes are not optimal from the hydrodynamic point of view.

In most cases, CDF calculations are consistent with our experimental results and the available literature data. However, in some comparisons, the differences are too great.

The existing differences in absolute values between simulation results and literature data require further experimental investigations. These are necessary to determine exact parameter values and to calibrate the computationally determined values by means of CDF simulations with the experimentally obtained ones.

Although much work has already been done in this field, our knowledge is still not complete. Yet, the very awareness of the existence of relationship between unit power input dissipation and apparatus geometry is particularly valuable in designing mixers for the crystallization process, especially with a chemical reaction or by salting out.

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