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NUMERICAL SOLUTION OF POPULATION BALANCE MODEL FOR NANO QUARTZ CRYSTALLIZATION

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KEYWORDS

Population balance model, crystallization, quartz, cyclone

ABSTRACT

The population balance model provides an appropriate mathematical framework for the modeling of crystal size distribution (CSD). In this paper we use computational fluid dynamics (CFD) for modeling quartz crystallization in the cyclone. The study of gas-phase changes leading to nucleation of the first solid particles has to be coupled with the study of the evolution of the particle distribution by solving a population balance equation via the Direct Quadrature Method of Moments (DQMOM).The Method used to produce nano-quartz particles is gas condensation. In this method, silica vapor with nitrogen gas at high temperatures mix with cold nitrogen gas and solid particles are quickly formed. Result predicted by Fluent show the formation of quartz nanoparticles in the cyclone.

INTRODUCTION

Nano-silica is a very important material for different industries such as cement and concrete. In this work we simulate crystallization of nano-silica by solving a population balance equation via the Direct Quadrature Method of Moments (DQMOM). These types of processes involve formation of entities, growth, breakage or aggregation of particles, and are, therefore, present in a large range of applications, like crystallization, polymerization, bubble towers, biological processes, aerosol reactors fermentation or cell culture [1-3]. This paper investigated the possibility of nanoparticles formation under defined conditions in the cyclone.

THEORY

The population balance equation in size coordinates (with L as a representative diameter of a particle) can be written in the form [4-5]:

$$\frac{\partial n}{\partial t} + \frac{\partial (Gn)}{dL} + n\frac{\partial V}{V \partial t} + D(L) - B(L) + \sum \frac{\dot{V}_i n}{V} = 0 \qquad (1)$$

The number density function is n, V is the number of particles per unit volume, in the crystal size interval dL. G is The growth rate of a single crystal, B(L) and D(L) are the birth & death rate of crystal. The DQMOM is based on solution of the following equations [6] :

$$\frac{\partial w_\alpha}{\partial t} + \frac{\partial}{\partial x_i}\left(\tilde{U}_i w_\alpha\right) - \frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial w_\alpha}{\partial x_i}\right] = a_\alpha \qquad (2)$$

$$\frac{\partial L_\alpha}{\partial t} + \frac{\partial}{\partial x_i}\left(\tilde{U}_i L_\alpha\right) - \frac{\partial}{\partial x_i}\left[\Gamma_t \frac{\partial L_\alpha}{\partial x_i}\right] = b_\alpha \qquad (3)$$

Where $L_\alpha = w_\alpha l_\alpha$, Γ_t, $w_\alpha(x,t)$, $\tilde{U}_i$, a_α and b_α indicate the αth weighted abscissa, turbulent diffusivity, weights, Favre-averaged value of the ith component of the fluid mean velocity, source terms respectively. The kth moment of the distribution can be written as [7]:

$$\tilde{m}_k(x,t) = \int_0^{+\infty} \tilde{n}(L;x,t) L^k \, dL \approx \sum_{\alpha=1}^{N} w_\alpha L_\alpha^k \qquad (4)$$

Where, number density function is n and dL is the crystal size interval. The zeroth moment represents the number of crystals per unit mass of solvent. The first moment is total length of all crystals per unit mass of solvent, the second and third moments are related to the area and the volume of crystals per unit mass of solvent respectively.

MODELING

The 3D volume grid is represented in Fig 1. In the optimal grid, the domain is discretized into a grid of 86732 tetrahedral cells. The conservation equations for mass, energy, momentum, Reynold's stresses and dissipation rate are solved by finite-volume analysis, using a first-order upwind scheme for discretisation of the convective terms in the transport equations.

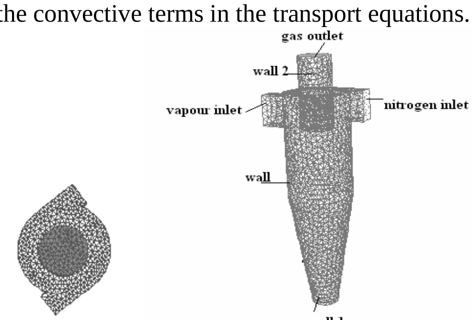


Figure 1. Three-dimensional tetrahedral grid

0.1 mole of quartz vapor at 2500 K with 0.9 mole of nitrogen gas are conducted to the first inlet and 2 moles of nitrogen gas at 356 K enter the second inlet of the cyclone. They mix and quickly cool and the silica nano-crystals are formed. Results predicted by the software also indicat similar trends.

RESULTS

Figure 2 – a and b show that the particle size of solid phase are related to mixture temperature and nanoparticles of quartz are formed in the cyclone.

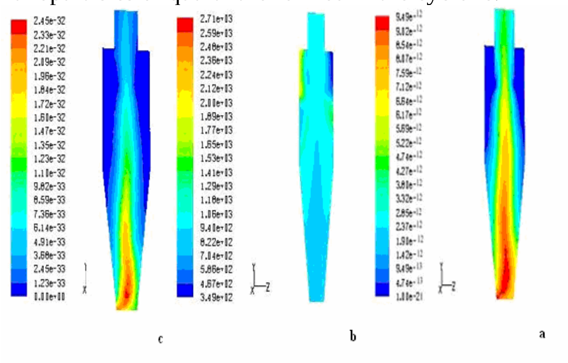


Figure 2: a)diameter range of solid phase b) temperature changes c) volume fraction of solid phase

The volume fraction of solid phase which is shown in part c of the figure, reveals that larger particles are produce in lower areas of the cyclone. Size distribution of particles according to position in the cyclone is shown in figure 3. The results of figure3 agree with figure 2.

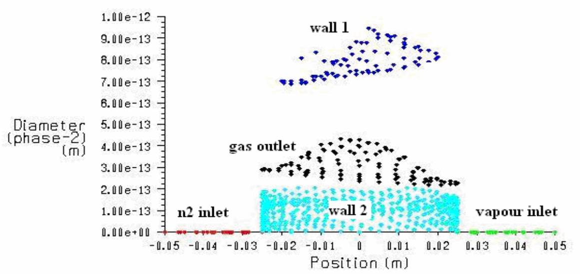
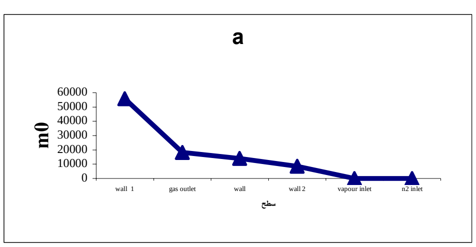


Figure 3: size distribution of particles according to position in cyclone

As we have seen, smaller particles under the centrifugal force of the cyclone have been thrown towards the wall. The amounts of 0-3th moments over different surfaces of the cyclone are shown in figure 4. As shown in figure, the number of crystals in the lower output and the higher input of cyclone reaches zero and accumulation of crystals in the bottom outlet of the cyclone causes it to reach maximum level of total length.



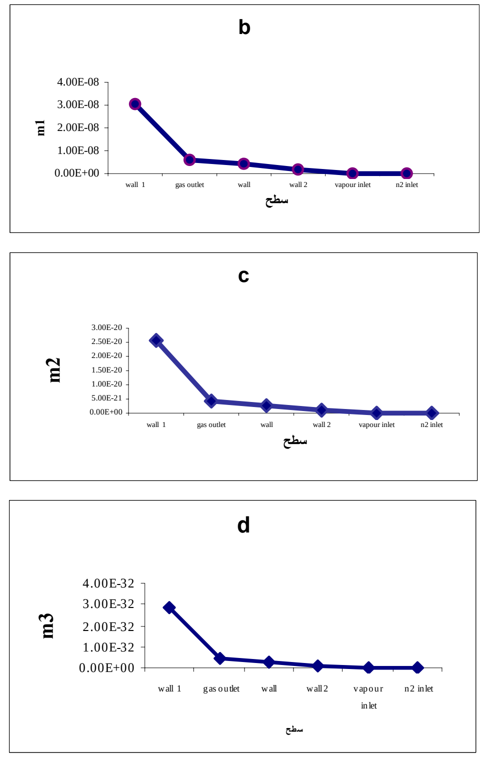


Figure 4: a) number of crystals per unit mass of solvent , b) total length of all crystals per unit mass of solvent, c) area per unit mass of solvent, d)volume of crystals per unit mass of solvent

Also, all the above charts represent a downtrend in which the maximum number, size and the crystal surface per unit mass of solvent are in the bottom outlet of the cyclone, the intermediate ones are on the wall and the minimum values are in the inlets. The predicted results show the formation of quartz nanoparticles in cyclone.

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