Physico-chemical models of glass melting

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The present role of mathematical models in glass melting involves acquisition of new knowledge, technology improvement and control, as well as develepment of new processes and preparation of new glassy materials. The partial models may be classified according to several point of views but the family of homogeneization models, involving physico-chemical descriptions of homogeneization processes and able to be combined into more complex models, seems to fulfil best the role of modeling. Such modular models may be used for a wide scale of glass technology tasks, are relatively transparent, adjustable and often fast in calculations. The presented classification includes three groups of models, single particle models, melt behavior models and distribution models. Every partial (modular) model is characterized by governing equations, limits of its application, necessary data for calculations and by combination opportunities with other models. The methods of data acquisition and verification of models are needed parts of the work. The purely experimental models or models with estimations of process kinetics describe process having too complicated or not sufficiently transparent course.

The models of single solid particles take into account diffusion and chemical reaction, being applicable for polydisperse particles. The until now applications included SiO_2 particle dissolution in glass, spinel crystal precipitation during vitrification of high level radioactive waste and qualitalive application leading to preparation of gold ruby glass. Single bubbles are described by two models, the complete one describing both the bubble size and composition developments and characterized by a considerable demand of data, and the simplified one, describing only the bubble size development on the base of relatively easy laboratory experiments. The second model is well usable for refinig studies, however, the identification of bubble sources by modeling needs to know also composition development of defect bubbles.

Different models of glass melt flow are applied according to purpore of investigation. Quiescent glass is chosen to describe results of laboratory measuremants, perfect mixing may be sometimes applied for vigorously stirred melting spaces, the piston flow was chosen for verification of distribution models while the 3D flow is generally applied to simulate melt behavior in real melting spaces.

Two particle distribution models are applied to calculate the concentration field of particles in melt. The model based on particle tracing is applicable when the melt and particles do not mutually influence, the second model, based on the convective transport of particle phase, was used to calculate bubble impact on glass flow in the model melting space. The distribution of components of oxidation-reduction reactions is needed to model bubble behavior under real conditions. Its reasonable application involes considering bubble impact on glass redox in regions with high bubble concentrations.

The model data acquisition into single models includes a wide class of laboratory techniques, the most problematic acquired values being at present data characterizing gas diffusion and dissolution in glasses. However, the mentioned gas data derived from laboratory bubble examination at melting temperatures seem to simulate well bubble behavior under real conditions.