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Silicon oxide flames and the formation of silica fume

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When producing silicon or ferrosilicon, silica fume is a major by-product. Up until the 1980s, this was an environmentally challenging side stream, but since then it has been turned into a valuable by-product due to its use in various advanced materials. It is particularly valuable because of its ability to significantly increase particle packing in refractory materials and its use as a pozzolan in concrete. Silica fume coming from silicon and ferrosilicon furnaces are amorphous, non-porous, spherical nanoparticles of almost pure silicon dioxide. When converting the furnace process from fossil-based to bio-based reducing agents, it is crucial that the quality of the silica fume is not degraded. It is therefore important to fully understand the mechanisms by which the silica fume particles are formed. This is the aim of the current work.

The gaseous silicon-dioxide that will eventually form the particles comes as a result of combustion of silicon-monoxide (SiO) that emerges from the furnace charge together with carbon-monoxide (CO). When the mixture of SiO and CO meet the air that flows into the furnace above the charge, it burns in an intense flame right above the charge. Since the boiling temperature of SiO_2 is relatively high (2230°C), SiO_2 molecules will start to nucleate into SiO_2 particles in the post-flame region. Molecular SiO_2 that is still in the gas phase will then condensate on these nuclei or generate new nuclei. In the temperature range above the melting point of quartz (1723 °C), silica fume particles that collide will coalesce to form larger particles.

We present results from detailed direct numerical simulations (DNS) of SiO/CO combustion in a triple-periodic temporal jet framework, and the resulting nucleation and condensation of SiO_2; see Figure 1 for an example. This is done by performing three-dimensional DNS of a small sub-volume of a real furnace, while incorporating all relevant physical and chemical effects, using the best available values for the relevant parameters. This is the first time such detailed simulations of this process are performed, and fundamental new knowledge about the formation process of silica fume is obtained. An example is the explosive chain reaction resulting from the high temperature sensitivity of the nucleation process and the liberation of the vaporization energy.

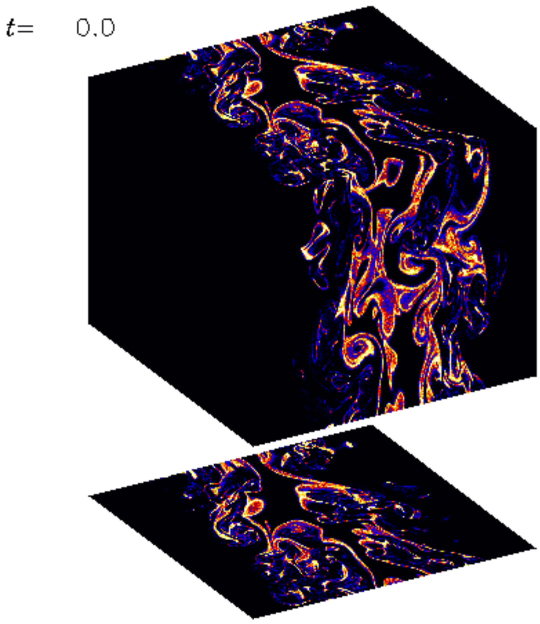

Figure 1: Silica fume particles in a turbulent temporal jet