

**Q1** What is your organisation's/project's name?

Chiesi farmaceutici

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**Q2** Your organisation's/project's website

<http://www.chiesigroup.com/>

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**Q3** Are you?

**A company**

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**Q4** Your name

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**Q5** Your email address

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**Q6** Your contact phone number

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**Q7** Please summarise who you are and what you do

Chiesi is an international pharmaceutical company with a focus on respiratory and rare diseases and neonatal care. As the R&D product and process development departments we formulate a targeted active molecule into a stable drug product to be tested in the early phase toxicological or clinical studies. Our work with the drug product process design continues with the scale-up from lab/pilot scale to industrial scale culminating in the delivery of a reproducible and robust manufacturing process to the production plant engineers. The kind of pharmaceutical forms we usually work with are dry powders for inhalation, tablets, solutions and suspensions which necessitates us dealing daily with problems of powder flow and rheology, powder milling and mixing, powder dissolution and dispersion in fluids, powder fluidization and powder compression. Formulating such kinds of drug products requires knowledge of the mechanical and chemical properties of the starting and intermediate materials as well as of the physical properties of the powders and powder-fluid mixtures when subjected to mechanical and thermal stresses. Our modelling activity (mainly DEM and CFD) is focussed on the understanding and improving of our formulation capabilities, production process design and optimization and product-process interaction.

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**Q8** In what way would like to contribute to an EsD project? **An an application provider**

**Q9** What would be your contribution to an EsD project?

As an application provider we can easily chart a number of technological processes involving powders and powder-fluid mixtures whose physics is highly non-linear thus demanding a predictive modelling/computational tool (DEM or DEM-CFD based) to foster our understanding of them and to promote a lower cost and faster process design, scale-up and optimization. Involving easily from many tens of million up to many billions particles, requiring a DEM-CFD coupling strategy whose algorithms must scale up to many hundreds of cores/gpus, we believe such kind of simulation activity might fit in a EsD project.

Having in-house all the instrumentation to characterize the material properties as well as the mechanical/rheological behaviour of powder, working directly with the production plants and machines involved in the manufacturing process we can provide, within a collaborative project, all the experimental data to calibrate model and interaction-potential parameters. We can then gather all the experimental data to assess the quality of the finished products as well as the statistics generated by the in process control and monitoring of the manufacturing process against which the qualitative/quantitative predictive powder of the simulations should be tested for some selected case studies.

We also have in-house the expertise for handling large calculations on HPC infrastructures so part of the production runs can be run directly by us.

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**Q10** What partners are you looking for?

Within an EsD project we would need two different kinds of support: a technology provider assisting us in the initial code enabling step, offering us support for the code installation/optimization and providing the necessary HPC resources; a technology provider with more academic expertise on the simulation of powder mechanics/physics able to undertake the coding of new algorithms, interaction potentials and subroutines if and when necessary for specific applications.

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**Q11** Please include links to any additional material.

none

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**Q12** Other comments/ideas

Respondent skipped this question

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