



## IFPRI BRIEF TEMPLATE

Check One:    **Project**                       **Review**                       **Collaboration**  
                    **Workshop**                       **Other**

<b>Descriptive Title</b>	<b>Effect of ultrasound (US) on crystallisation mechanisms (nucleation and breakage) and crystal properties (size and polymorphism)</b>
<b>Working Title<sup>1</sup></b>	Sonocrystallisation
<b>Technical Area<sup>2</sup></b>	F, SR
<b>Date</b>	14/06/2022
<b>Short Description</b>	Sonocrystallisation is the use of ultrasound to aid crystallisation process. Although there are general understandings on the effect of ultrasound (US) on crystallization, such as reduced induction time and metastable zone, increased nucleation rate which lead to smaller crystals with a narrower size distribution when compared with conventional crystallizations, the prediction and design of sono-crystallisation is more an art than a science. There is a lack of mechanistic and systemic approaches in the design of sono-crystallizer, with limited knowledge on how the key US parameters such as frequency are related to the nucleation rate and breakage, as well as the key crystal properties such as crystal size and polymorphs. In addition, most literature focuses on continuous sonication over the entire crystallisation time with limited US frequency used (mostly 20kHz), but two reports have shown short bursts of ultrasound is sufficient to create the sonocrystallisation benefits. This would be a more effective use of ultrasound and useful for scaling up sonocrystallisers.
<b>Objectives</b>	Understand and quantify the effect of ultrasound parameters (frequency and power, continuous sonication vs pulsing) on the major crystallisation mechanisms, namely nucleation and breakage so that the key crystal properties such as crystal size and polymorphism can be predicted.
<b>Scope</b>	Two model compounds with polymorphs will be selected. The proposed project scope is: (1) Sono-fragmentation: Experimental investigation using breakage only sonocrystallizer and <b>in line</b> crystal size measurement to measure the effect of US parameters (wide

<sup>1</sup> Title used in meeting agendas and file archives

<sup>2</sup> One or more from the following list: W = wet systems; D = dry systems; F = particle formation; SR = size reduction; M = modeling; SE = systems engineering

	<p>range of frequency and power) on breakage at different sonocation conditions. Breakage models will be developed and validated;</p> <p>(2) Nucleation rate, crystal size and shape: Through in line crystal size distribution measurement in a sonocrystalliser and the breakage model developed in scope (1), the crystal size model based on the population balance framework will be developed so that both the nucleation and growth rate parameters in the model will be related to US conditions</p> <p>(3) Experimental investigation: Pulsing versus continuous US, with real time crystal size and shape logging so that the best mode of US operation can be determined</p> <p>(4) Scaling up recommendations based on US power density</p>
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<b>Recommended Contractors (2 or 3)</b>		
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