



**HAL**  
open science

## Modelling and simulation of particle milling in a stirred tank using CFD-PBE coupled approach

Zoé Mercier, Maxime Pigou, Pascal Fede, J-P. Bayle, Eric Climent, E. Tronche

### ► To cite this version:

Zoé Mercier, Maxime Pigou, Pascal Fede, J-P. Bayle, Eric Climent, et al.. Modelling and simulation of particle milling in a stirred tank using CFD-PBE coupled approach. 18th European Mechanics of Materials Conference (EMMC18), Apr 2022, Oxford, United Kingdom. cea-04743538

**HAL Id: cea-04743538**

**<https://cea.hal.science/cea-04743538v1>**

Submitted on 18 Oct 2024

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Welcome to EMMC18

## 18th European Mechanics of Materials Conference

April 4th-6th, 2022, Oxford

### Modelling and simulation of particle milling in a stirred tank using CFD-PBE coupled approach

The logo for CEA (Commissariat à l'énergie atomique et aux énergies alternatives) features the lowercase letters 'cea' in a white, sans-serif font, positioned above a thin green horizontal line.

DE LA RECHERCHE À L'INDUSTRIE

**Z. Mercier<sup>1,2</sup>, M. Pigou<sup>1</sup>, P. Fede<sup>1</sup>, JPh. Bayle<sup>2</sup>, E. Climent<sup>1</sup>, E. Tronche<sup>2</sup>**

<sup>1</sup> Institut de Mécanique des Fluides de Toulouse (IMFT), Université de Toulouse, CNRS, Toulouse, France

<sup>2</sup> CEA, DES, ISEC, DMRC, Univ Montpellier, Marcoule, France



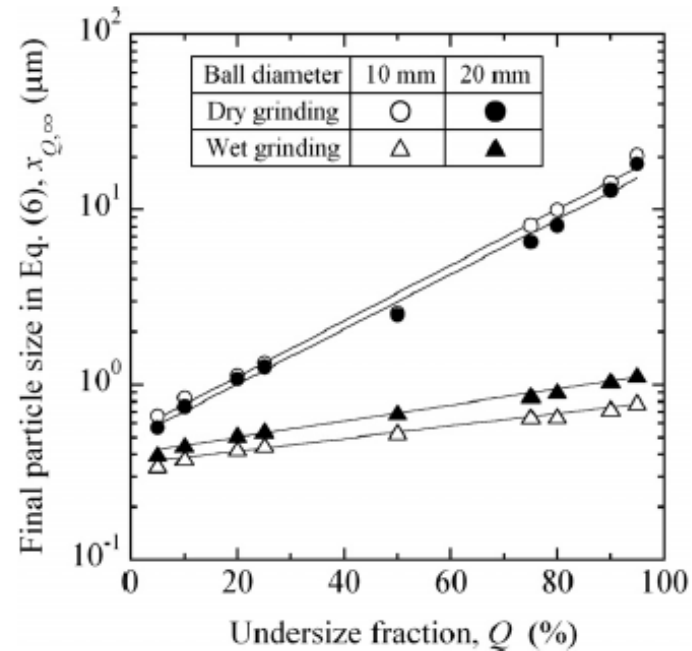
The demand for fine or ultra-fine particles is increasing in many industrial fields (ceramics, composite material, surface treatment...)

**Milling process** and **operating parameters** (angular velocity, grinding media properties...) have a great influence on **the size and the shape of the milled particles**.

### Experimental condition :

*N.Kotake et al 2011*

Quartz monodisperse particle milled in a laboratory scale mill  
Grind media : alumine balls (2 different diameters)  
Water is used for wet grinding



### Experimental conclusions :

- The product size in wet grinding is about ¼ the size in dry grinding
- The distribution is narrower for wet grinding
- Using small beads produces the minimal particle size distribution for the wet grinding but the maximal size distribution for dry grinding (compared with bigger beads)
- After 16h of dry milling there is no more breakage while for wet grinding particles still break after 128h

**Problem encountered : don't clearly understand operating parameter influence, thus controlling particle size distribution could be difficult**

## Aim : Modelling and simulated wet milling in order to determine the influence of operating parameters

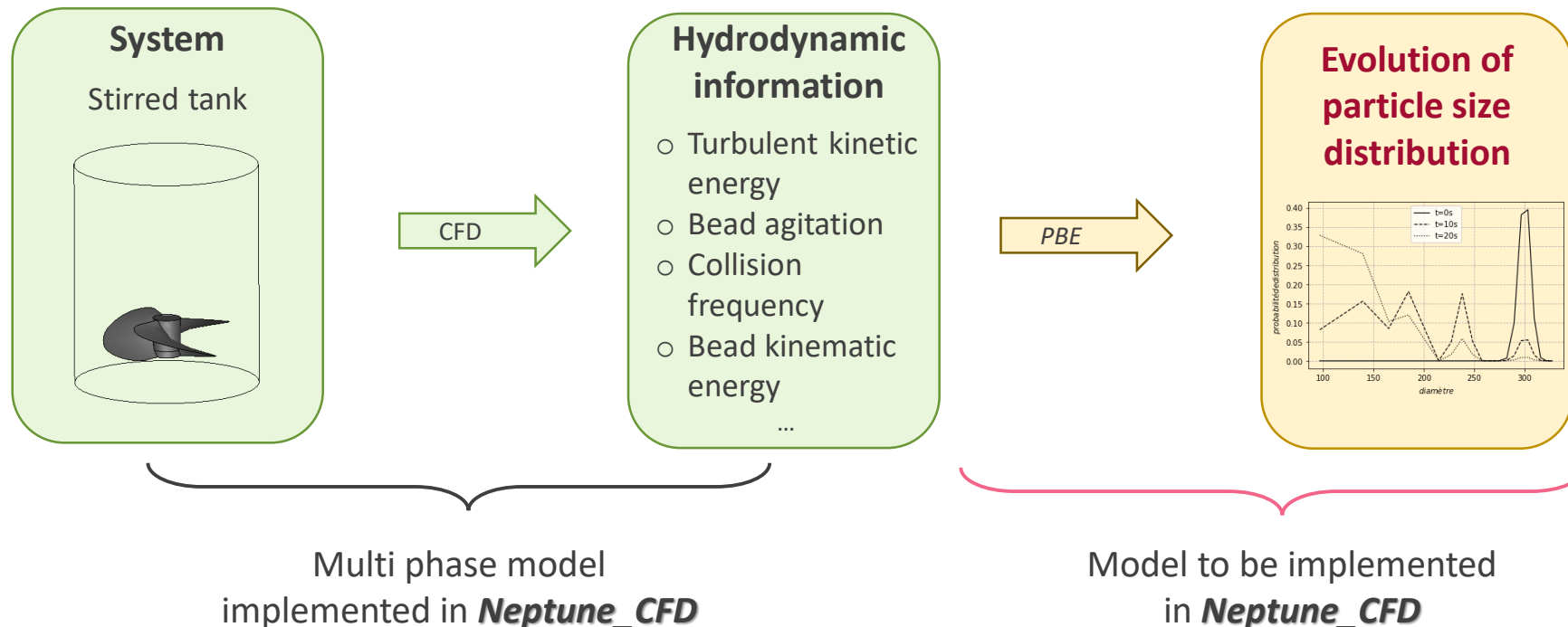
### Model Literature review of wet grinding

- Phenomenological model of grinding (SI-SN model).
- Computational Fluid Dynamics (CFD) and population balance equation (PBE) simplified coupled approach (using mean values of the flow)

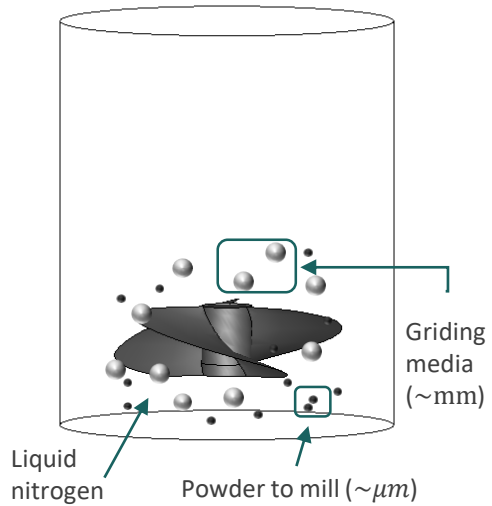
*E. Bilgili et G. Guner, 2020; Kwade, 1999.*

*Does not take into account local properties of the system (of the flow, of the distribution of the powder inside the tank...)*

### Method considered : CFD and PBE coupled approach

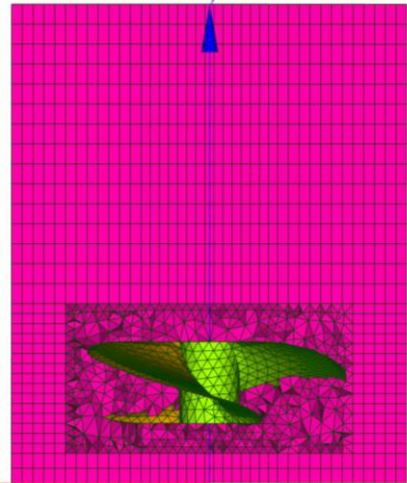
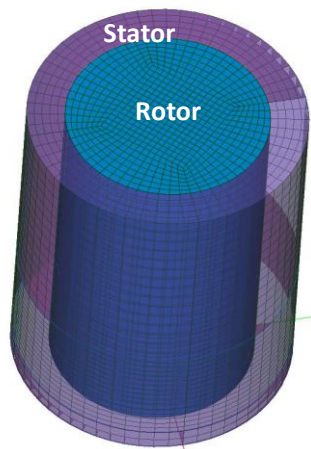
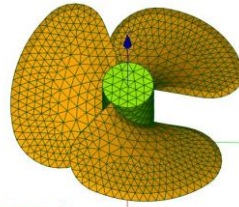


## System



Laboratory-scale: stirred tank with a boat impeller

- Volume:  $2.10^{-4}m^3$
- Mesh: 88 000 cells
- Angular velocity  $\omega = 600rpm$
- Rotor-Stator method



## Model

Two-phase model (Euler-Euler method)

## ❖ Mixture phase

## Continuous phase

Equivalent fluid model for the carrying fluid ( $f$ ) (liquid nitrogen) and particles to mill ( $p$ ) (Batchelor & Green viscosity model)

$$\mu_M = \mu_f \left( 1 + \frac{5}{2} \alpha_p + 6,95 \alpha_p^2 \right)$$

Turbulence model :  $k - \epsilon$

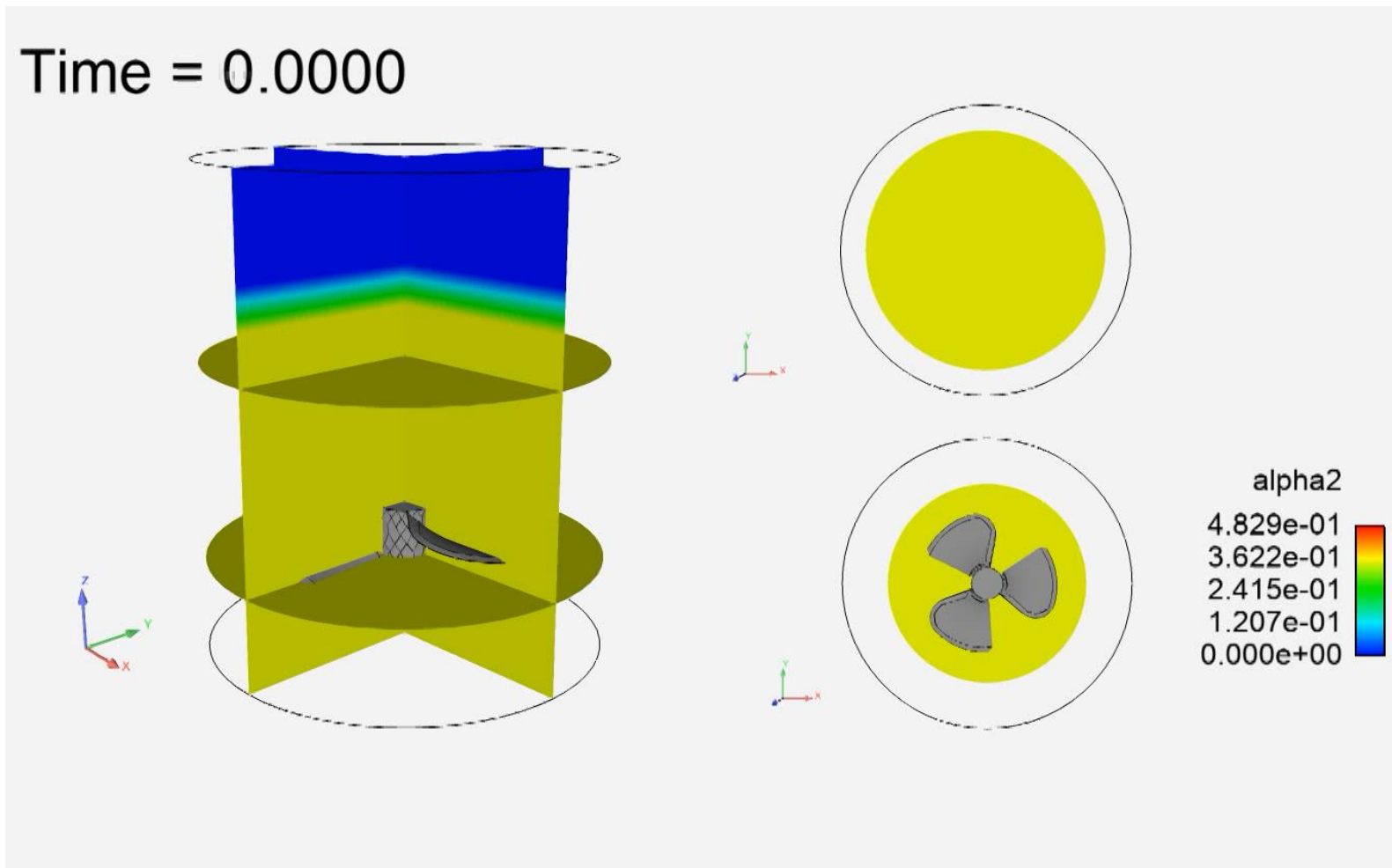
## ❖ Grinding media phase

## Dispersed phase

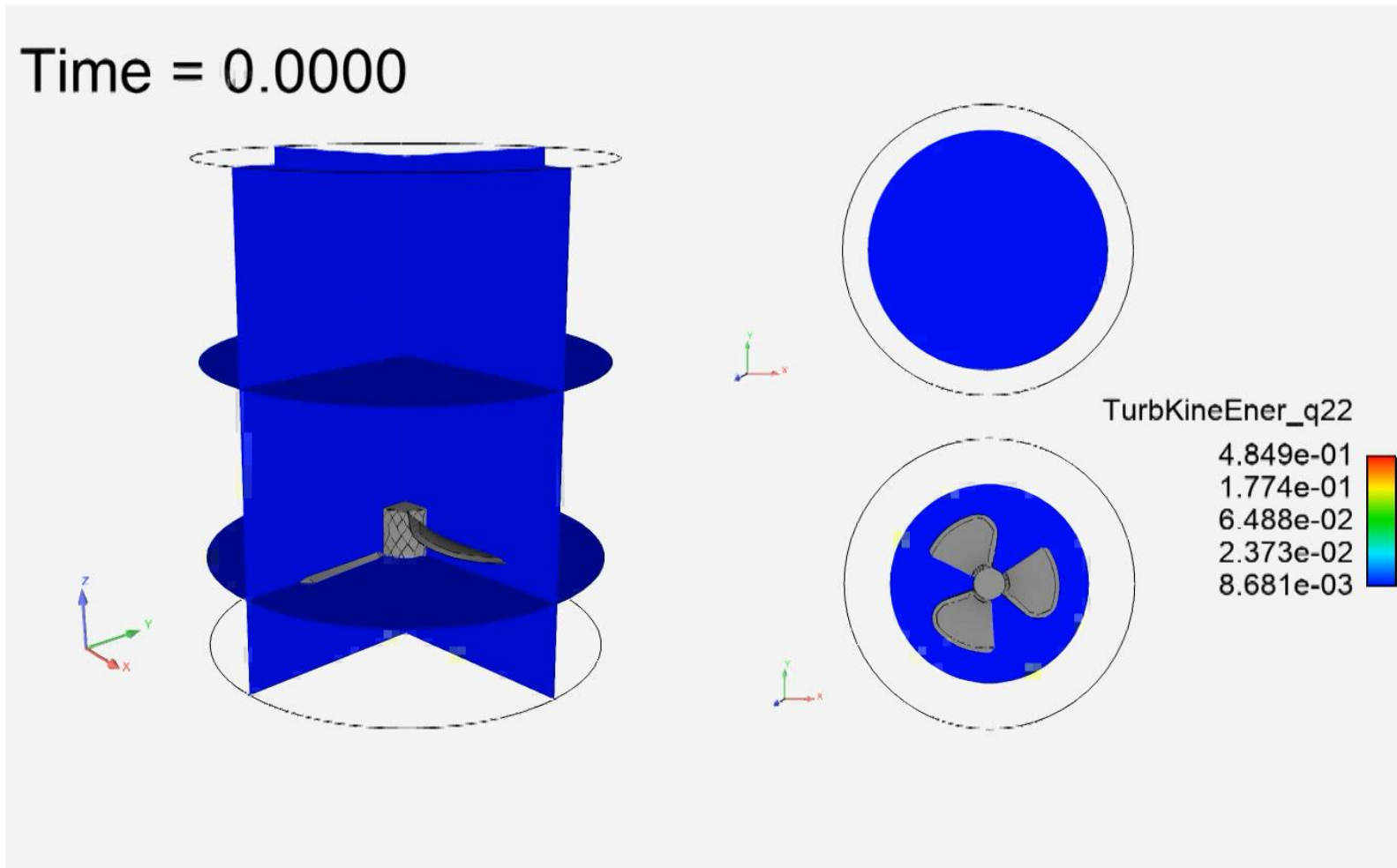
Spherical zircon beads

Turbulence model :  $q_p^2 - q_{fp}^2$

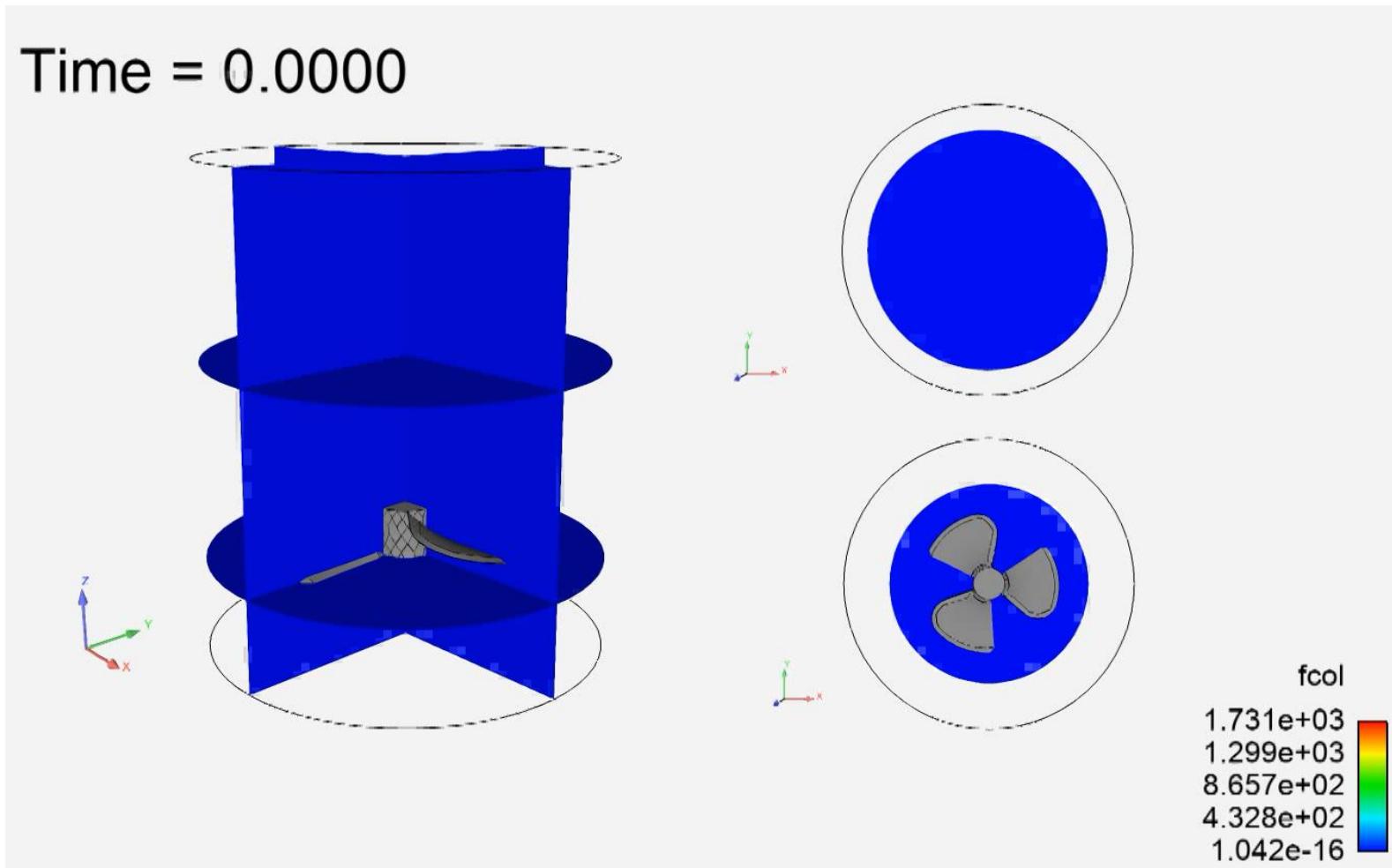
	Mixture	Bead
Viscosity $\mu$ (Pa. s)	$2.10^{-4}$	
Density $\rho$ ( $kg/m^3$ )	802	6520
Diameter $d_b$ (mm)		5
Volumic fraction $\alpha$	0.65	0.35



*Volume fraction of grinding media*



*Grinding media agitation*



*Grinding media collision frequency*



Population balance equation in terms of number density function  $n(v; \mathbf{x}, t)$

S. Castellano, 2019.

$$\frac{\partial n(v; \mathbf{x}, t)}{\partial t} + u \nabla n(v; \mathbf{x}, t) = S(v; \mathbf{x}, t)$$

Source term

$$S(v; \mathbf{x}, t) = B(v; \mathbf{x}, t) - D(v; \mathbf{x}, t)$$

Gain of a  $v$  volume particle

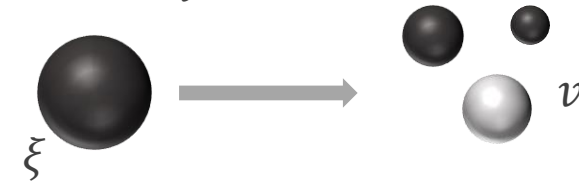
Loss of a  $v$  volume particle

Source term  $S(v; \mathbf{x}, t)$

Assumption: particles are only experiencing **breakage**

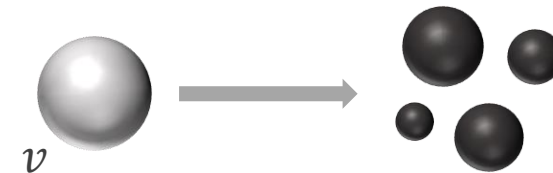
Birth term

$$B(v; \mathbf{x}, t) = \int_v^\infty k(\xi; \mathbf{x}, t) \beta(\xi, v) n(\xi; \mathbf{x}, t) d\xi$$



Death term

$$D(v; \mathbf{x}, t) = k(v; \mathbf{x}, t) n(v; \mathbf{x}, t)$$



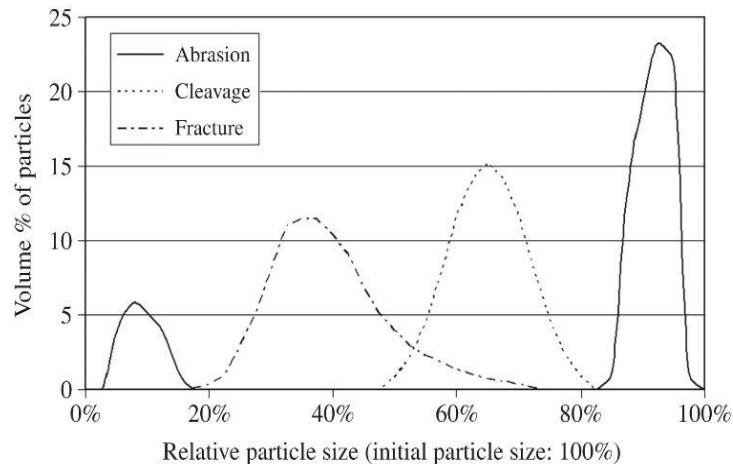
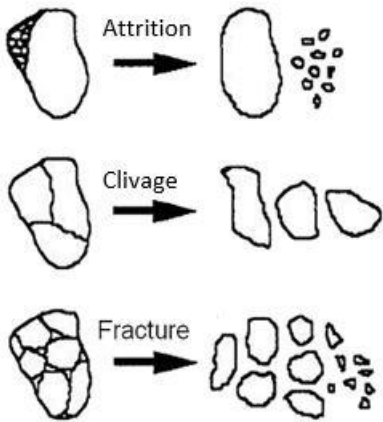
$k$  breakage kernel – how often a particle breaks ?

$\beta$  fragmentation distribution function – how a particle breaks ?

How a particle breaks ?

Different types of rupture

- Attrition when the particle is sheared
- The cleavage during a compression
- Fracture on impact



Fragmentation distribution function  $\beta$  models the type of rupture

Experimental method chosen :

Powder wet milling

Laser diffraction mesure

Particle size distribution

PBE Kapur approximation  
PC Kapur.1970

$B_{ij}$  values (class discretisation applied to  $B$  the cumulative distribution of  $\beta$ )

$$B_{ij} = \phi \left( \frac{x_{i-1}}{x_j} \right)^\gamma + (1 - \phi) \left( \frac{x_{i-1}}{x_j} \right)^\alpha$$

$\phi, \gamma, \alpha$  adjust parameters (depend only on particle not of the system considered)

LG Austien et al 2007

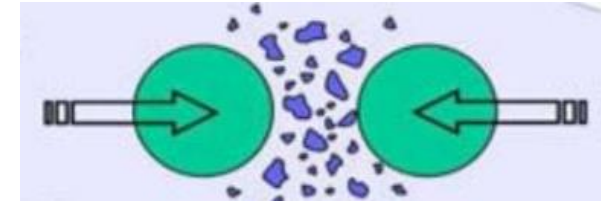
$\beta$  function

Statement to be validated  
adjust parameters will be determined for different operating parameters

How often a particle breaks?

Hypothesis : particles break because of bead/bead collisions only

*KWADE, Arno Powder Technology, 1999*



$$k(\xi; \mathbf{x}, t) = \text{bead collision frequency} * \text{capture probability} * \text{breakage probability}$$

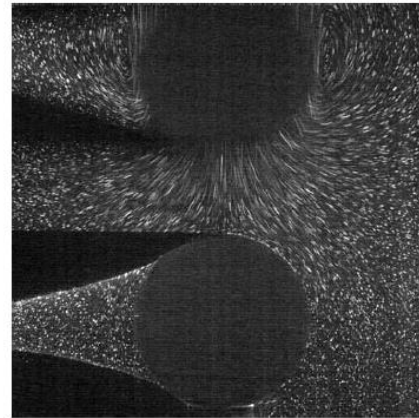
When two beads collide some particles go out the capture zone

### Frontal collision experimental study

*GERS R 2009 (Thèse de doctorat)*

Capture probability increases with particle inertia (bead approach velocity  $V_a$ , particle size  $D_p$ )

		$V_a$ (mm/s)	
		10	3.5
$D_p$ ( $\mu\text{m}$ )	280	2.37%	1.43%
	28	1.05%	1.04%



CFD output

A collision should be enough powerful to lead to breakage

$$P_b = 1 - \exp[-f_{MAT} D_p (E - E_{min})]$$

$E$  energy available for the breakage  
 $D_p$  particle size } CFD output

$E_{min}$  minimal energy needed to break  
 $f_{MAT}$  particle property } Particle properties  
 Experimental studies ?

*VOGEL, L. et PEUKERT. Powder Technology, 2003.*

## System input

Angular velocity $\omega$	600
---------------------------	-----

## Phase properties

	Mixture	Bead
Viscosity $\mu$ (Pa. s)	$2.10^{-4}$	
Density $\rho$ ( $kg/m^3$ )	802	6520
Diameter $d_b$ (mm)		5
Volume fraction $\alpha$	0.65	0.35

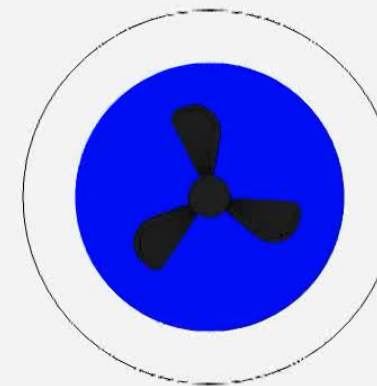
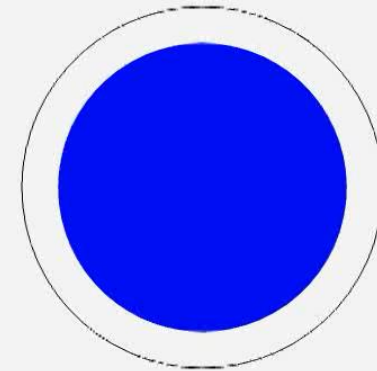
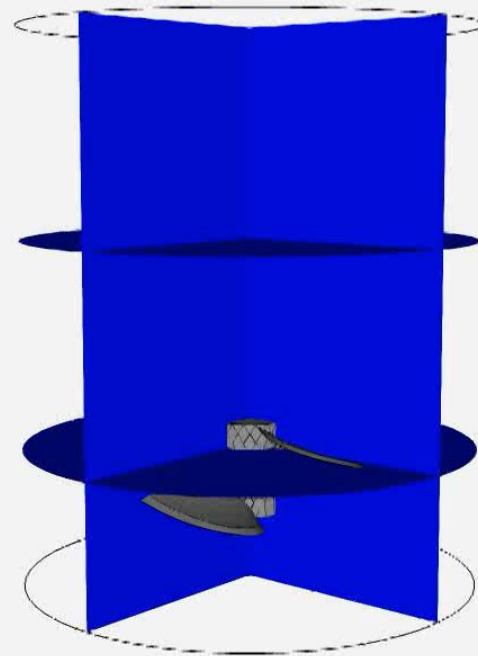
## Breakage hypothesis

Breakage kernel $k$	Bead collision frequency
Fragmentation distribution function $\beta$	Binary symmetric fragmentation

## Species parameters

Number classes $N$	10
Particle volume fraction $Y_p$	0.10
Initial volume (monodisperse distribution) $V_0$ ( $m^3$ )	$1,27e^{-9}$

Time = 0.00000



rapport\_vol  
 1.000e+00  
 7.563e-01  
 5.125e-01  
 2.688e-01  
 2.505e-02



## Conclusion

- ▶ CFD and PBE have been coupled in Neptune\_CFD software
- ▶ A first study has been carried out and gives a first approximation (assumptions: breakage kernel equal to bead frequency collision, binary symmetric collision)

## Perspectives

- ▶ **Breakage model development**
  - Breakage kernel  $k(v; x, t) = f_{coll} * capture\ probability * collision\ efficacy$
  - Fragmentation distribution function  $\beta$  : experimental studies
- ▶ **Experimental studies planned to validate the model**



Thank you for your attention

