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METAMODELS FOR CALIBRATING THE FRICTION COEFFICIENTS IN A ROTARY DRUM FROM DEM SIMULATIONS

Marcela V. C. MACHADO¹, Artemio PLANA-FATTORI¹, Kevin LACHIN¹, Stephane VITU^{1,2}, Cristian TRELEA¹, Mikel LETURIA³, Elias DAOUK³, Khashayar SALEH³, Marie DEBACQ^{1,2}

¹Université Paris-Saclay, INRAE, AgroParisTech, UMR SayFood, 91120, Palaiseau, France.

²Conservatoire National des Arts et Métiers (CNAM), 75003, Paris, France.

³Université de Technologie de Compiègne, ESCOM, TIMR, Centre de Recherche de Royallieu, Compiègne, France.

1 - Introduction

Rotary drums

- Particulate systems + fluids
- Isothermal or non-isothermal
- A large number of industrial processes: rotary kilns, dryers, mills, etc
- **But lack of simple tools for the industry**

Experimental



Modeling

- Dimensioning of process variables
- Materials properties

- Understanding the flow material behavior with more details
- Overcoming industrial safety limitations

Discrete Element Method (DEM):

Requires the specification of input parameters related to the particle properties and particle-particle (PP) and particle-wall (PW) interactions.

CALIBRATION STEP: adjusting the parameters until the model response corresponds to the equivalent experimental responses.

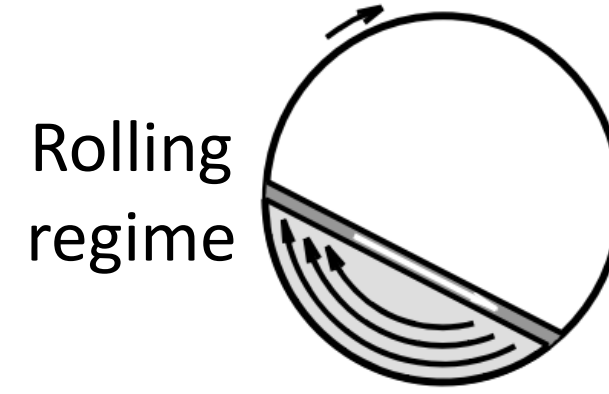
Problem in this approach:

Possibility of non-unicity in the set of parameters.

2 - Goals

- ❖ To study the influence of static friction (SF) and rolling friction (RF) coefficients in both interactions particle-particle (PP) and particle-wall (PW) on the dynamic repose angle of quinoa seeds in a rotary drum.
- ❖ To obtain metamodels, which allow analyzing the interaction between the parameters and their significance.
- ❖ To validate the four parameters set found in other speed rotations.

Figure 1:



3 - Methodology

3.1. DIRECT COMPUTATION

Lagrangian Method or Discrete Element Method (DEM):

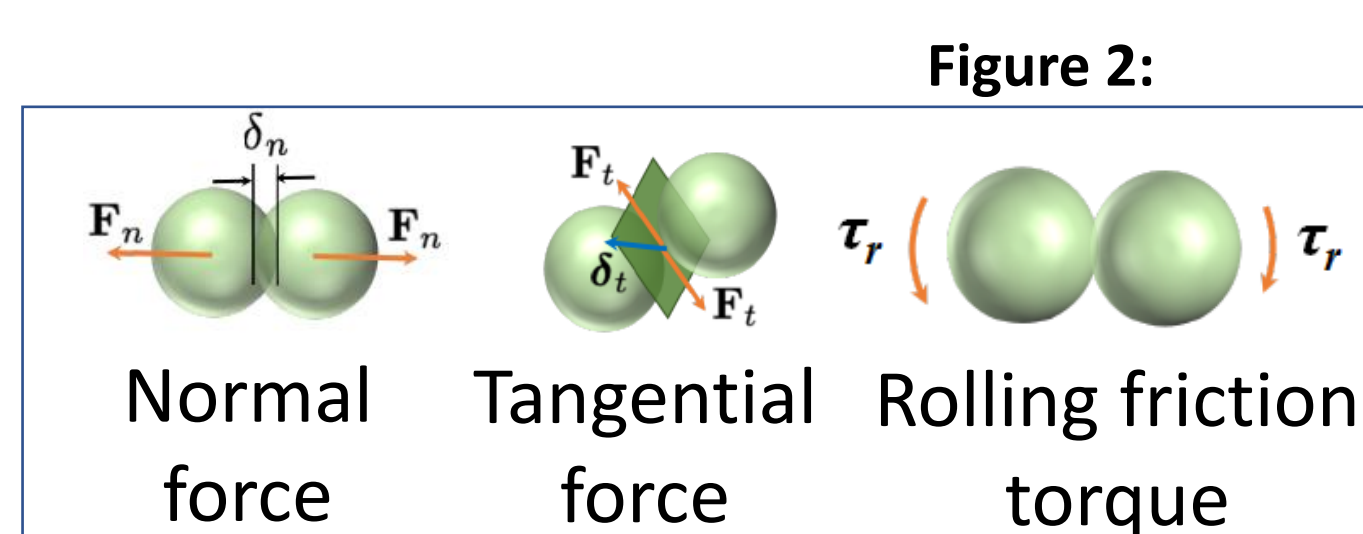
- All the particles trajectories are tracked.
- Temporal integration is applied to each of them using Newton's laws:

$$\text{Translation: } m_i \frac{dv_i}{dt} = \sum_j (F_n^{ij} + F_t^{ij}) + m_i g$$

$$\text{Rotation: } I_i \frac{d\omega_i}{dt} = \sum_j (R_i \times F_t^{ij}) + \tau_{ij}$$

$$\text{Normal force: } F_N = \lambda_{AN} v_{Nij} - k_N \delta_N$$

$$\text{Tangential force: } F_T = \begin{cases} \mu_p F_N, & \text{se } |F_T| \leq \mu |F_N| \\ \lambda_{AT} v_T - k_T \delta_T, & \text{se } |F_T| > \mu |F_N| \end{cases}$$



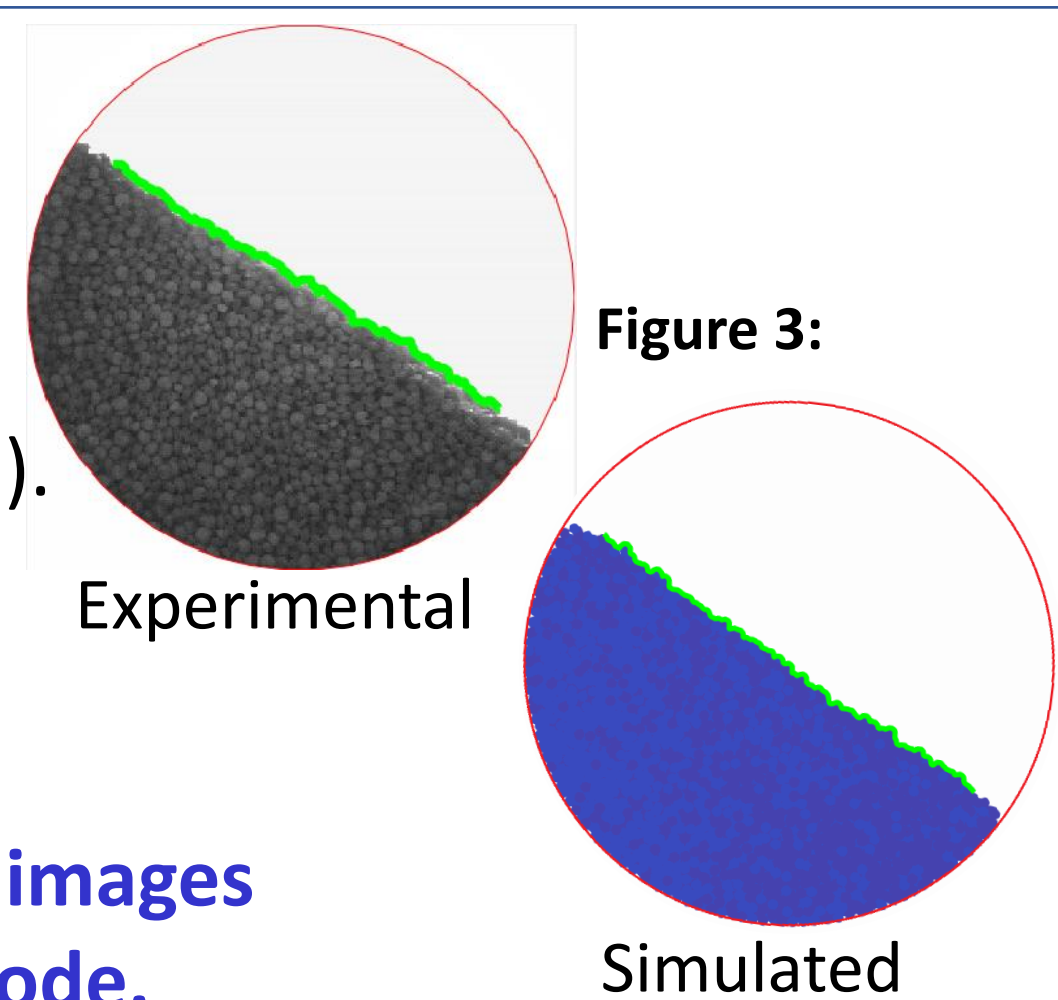
Fang, L., Zhang, R., Heuvel, C.V., Serban, R., Negrut, D. (2021). Processes, 9, 1813.

$$\text{Torque: } \bar{\tau}_{ij} = -\mu_R \bar{F}_N R_i \bar{\omega}_i$$

μ_p : Static friction coefficient (SF)
 μ_R : Rolling friction coefficient (RF)

3.2. MODEL PARAMETERS

- Drum: diameter 0.084m and length 0.020m.
- Quinoa seeds: $d = 0.0017\text{m}$, $\rho = 1058 \text{ kg/m}^3$.
- Speed rotation: 6, 8, 10, 12 rpm (rolling regime).
- Time-step = $8.6 \times 10^{-6} \text{ s}^{-1}$ (5% of Rayleigh time).
- Software: LIGGGHTS®.



- **Linear regression in the mean interface of 200 images of the bed drum, implemented by a MATLAB code.**

3.3. PARAMETERS IDENTIFICATION

(1) 4 Central Composite Designs: parameters: SFPP, SFPW, RFPP, RFPW 26 simulations for each speed rotation.

(2) 4 metamodels: verification of the interactions between the parameters.

(4) Validation: Comparison: angles calculated by metamodels, angles simulated with parameters optimized, and angles measured experimentally.

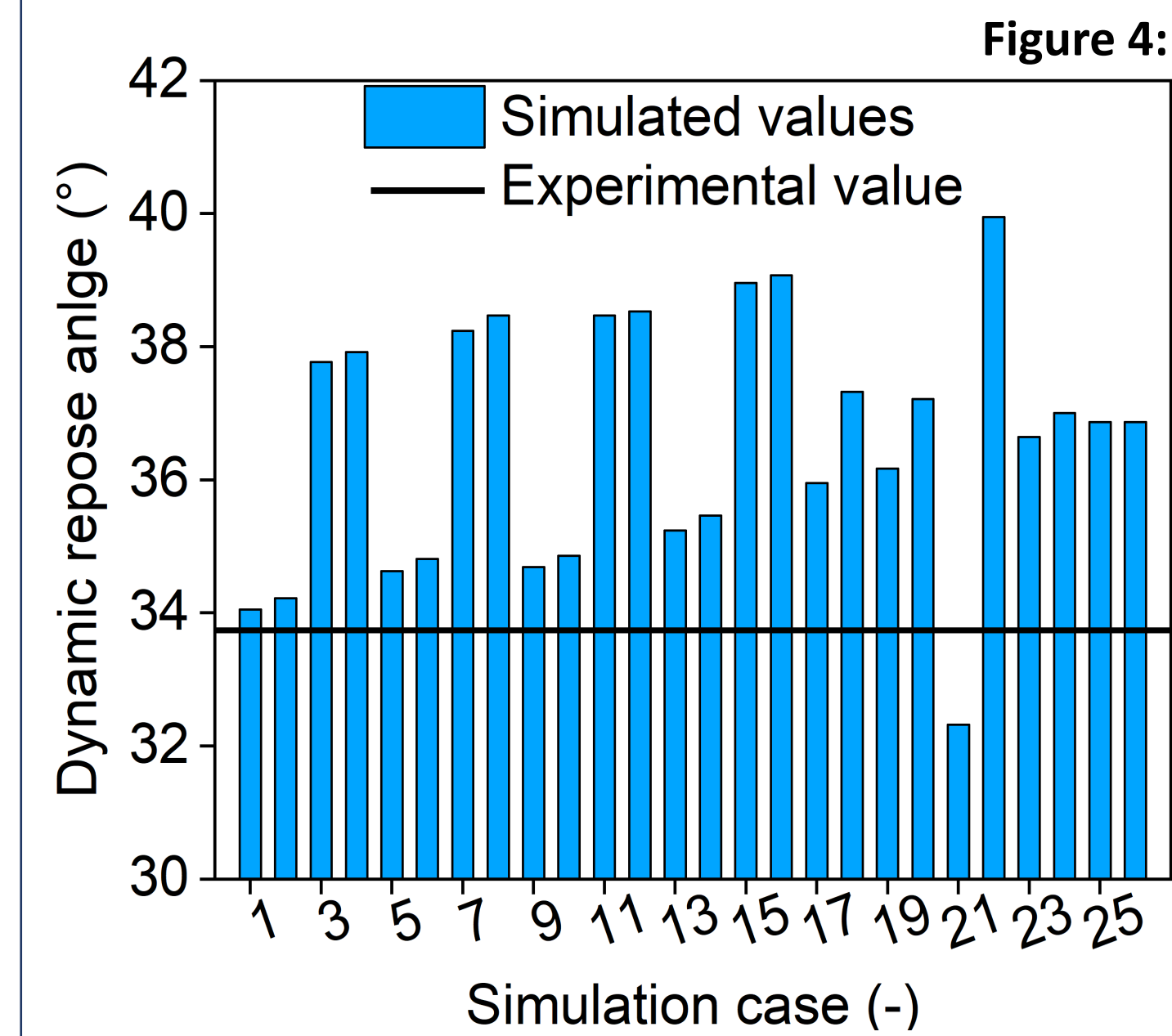
(3) Optimization: resolution of the metamodels and determining the 4 parameters optimized.

4 - Experimental and simulation results

4.1. Experimental dynamic angles of repose

Speed rotation	6 rpm	8 rpm	10 rpm	12 rpm
Angle (°)	31.96	32.46	33.14	33.74

4.2. Central Composite Design (CCD)



at 12 rpm:

Variable	Coded levels				
	-α	-1	0	+1	+α
SF PP	0.300	0.350	0.400	0.450	0.500
SF PW	0.350	0.400	0.450	0.500	0.550
RF PP	0.005	0.070	0.135	0.200	0.265
RF PW	0.300	0.350	0.400	0.450	0.500

α : axial points

- The rolling friction influence more on the dynamic angle of repose than the static friction, mainly in PP interactions, because it allows particles roll over each other, enabling better rearrangement and redistribution of stress, leading to a more stable packing.

4.3. Metamodels estimated for the dynamic angle of repose (°): (4 equations and 4 variables)

Metamodel at 12 rpm: $R^2 = 0,9995$

$$\Theta = 20,13 + \underline{x}'a_1 + \underline{x}'A_1\underline{x}$$

$$a_1 = \begin{bmatrix} 23.08 \\ 18.98 \\ 39.95 \\ 1.68 \end{bmatrix}, A_1 = \begin{bmatrix} -20.61 & 0 & 0 & 0 \\ 0 & -15.11 & 0 & 0 \\ 0 & 0 & -41.78 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \underline{x} = \begin{bmatrix} SF PP \\ SF PW \\ RF PP \\ RF PW \end{bmatrix}$$

Metamodel at 10 rpm: $R^2 = 0,9988$

$$\Theta = 20,32 + \underline{x}'a_1 + \underline{x}'A_1\underline{x}$$

Metamodel at 8 rpm: $R^2 = 0,9991$

$$\Theta = 20,75 + \underline{x}'a_1 + \underline{x}'A_1\underline{x}$$

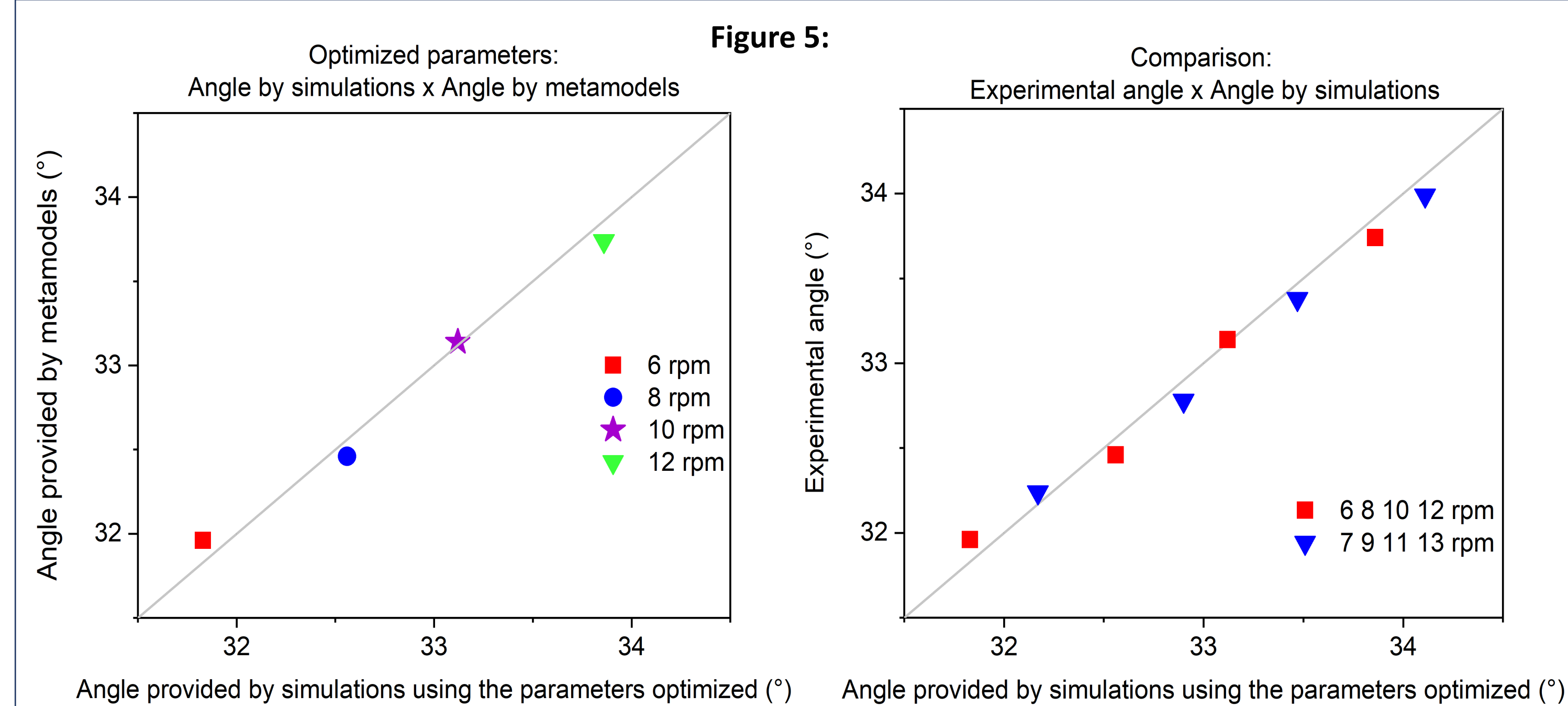
Metamodel at 6 rpm: $R^2 = 0,9935$

$$\Theta = 23,58 + \underline{x}'a_1 + \underline{x}'A_1\underline{x}$$

4.4. Optimization of the 4 metamodels and a single set of parameters with physical meaningful is found

	Angle Exp	Angle Model	% error
SF-PP 0.3226	6 rpm 31.96	31.83	0.4%
SF-PW 0.3938	8 rpm 32.46	32.56	0.1%
RF-PP 0.0665	10 rpm 33.14	33.12	0.3%
RF-PW 0.4227	12 rpm 33.74	33.86	0.4%

4.5. Validation: comparison between angles provided by metamodels, angles simulated with parameters optimized, and angles measured experimentally



5 - Conclusions and perspectives

- ❖ The DEM provides a good representation of the phenomenon, allowing a satisfactory visualization, in Figure 3 (experimental and simulation comparison);
- ❖ The metamodels estimated can reliably predict the angle of repose values for the range of parameters studied;
- ❖ The set of parameters optimized by metamodels predicted simulated angle values very close to the experimental values (< 1%) in all considered speed rotations;
- ❖ **NEXT STEPS:** to validate the set of parameters in a mixing assessment.

Contact:

Marcela V.C. MACHADO, Postdoctoral researcher, INRAE
marcela.vieira-caixeta-machado@inrae.fr



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Lina CAYLA (UTC, Compiègne)

