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**Title:**

In silico prediction of INFOGEST gastric phase hydrodynamics

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**Abstract:** (Your abstract must use **Normal style** and must fit in this box. Your abstract should be no longer than 300 words. The box will ‘expand’ over 2 pages as you add text into it.)

**Preparation of Your Abstract**

1. The title should be as brief as possible but long enough to indicate clearly the nature of the study. Capitalise the first letter of the first word **ONLY** (place names excluded). No full stop at the end.

2. Abstracts should state briefly and clearly the purpose, methods, results and conclusions of the work.

Introduction: Clearly state the purpose of the abstract

Methods: Describe your selection of observations or experimental subjects clearly

Results: Present your results in a logical sequence

Discussion: Emphasize new and important aspects of the study and conclusions that are drawn from them

“In vitro” digestion models are increasingly used to estimate reaction kinetics and bioavailability, and INFOGEST protocols have become the gold standard for experiment design. Semi-dynamic models strike a balance between the dynamic nature of the digestion process and experimental cost / feasibility. Continuous stirring is intended to homogenise digesta but how effectively this is achieved has not yet been investigated sufficiently and existing INFOGEST protocols provide little guidance for selecting optimal agitation controls. Within samples, non-physiological regions of poor transport and incomplete mixing may bias “in vitro” predictions. For gastric protocols, well controlled advective-diffusive mixing is important to ensure sufficient concentrations of enzymes and acid throughout the digesta to maintain effective reaction kinetics for protein and lipid hydrolysis.

We present here the first “in silico” assessment of digesta hydrodynamics for the combination of INFOGEST helical stirrer and conical titration vessel. Smoothed Particle Hydrodynamic (SPH) simulations are used to predict dispersive transport of injected gastric fluid and enzymes at different viscosities and fill levels. To do this, we simulate three timepoints across a semi-dynamic gastric phase protocol for a low viscosity liquid food [1].

Simulation predictions provide encouraging evidence that the combination of INFOGEST stirrer and titration vessel can produce a similar extent of spatially inhomogeneous flow and hydrolysis as exists “in vivo”. We found digesta viscosity to be an important control for how quickly and how completely injected enzymes and acid disperse. This suggests slower digestion of higher viscosity content early in the gastric phase (due to the presence of unmixed regions hindering digestion and nutrient bioaccessibility) as intended in the semi-dynamic protocol.

1. Mulet-Cabero, A. I., Egger, L., Portmann, R., Ménard, O., Marze, S., Minekus, M., ... & Mackie, A. (2020). A standardised semi-dynamic in vitro digestion method suitable for food—an international consensus. *Food & function*, 11(2), 1702-1720.