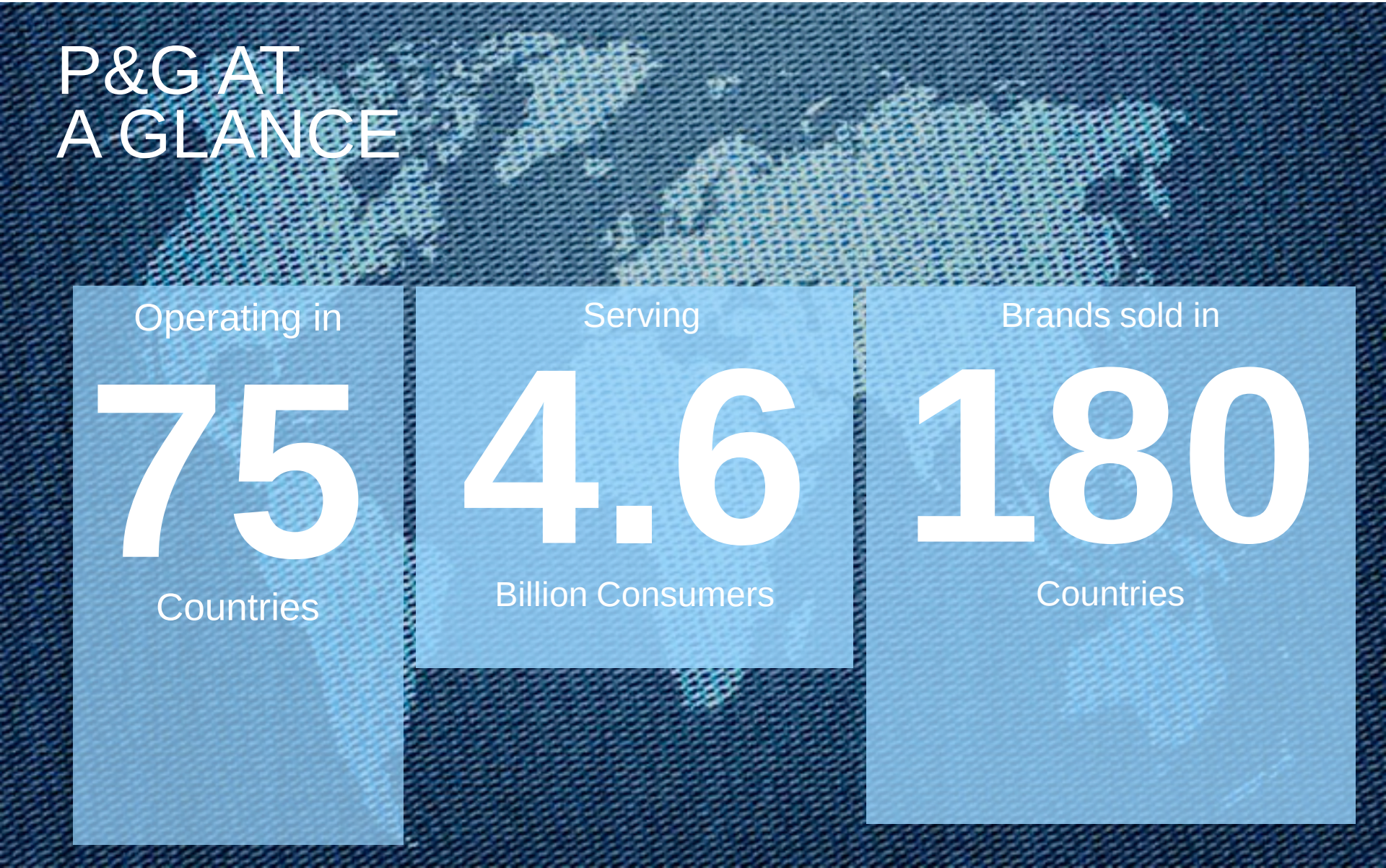
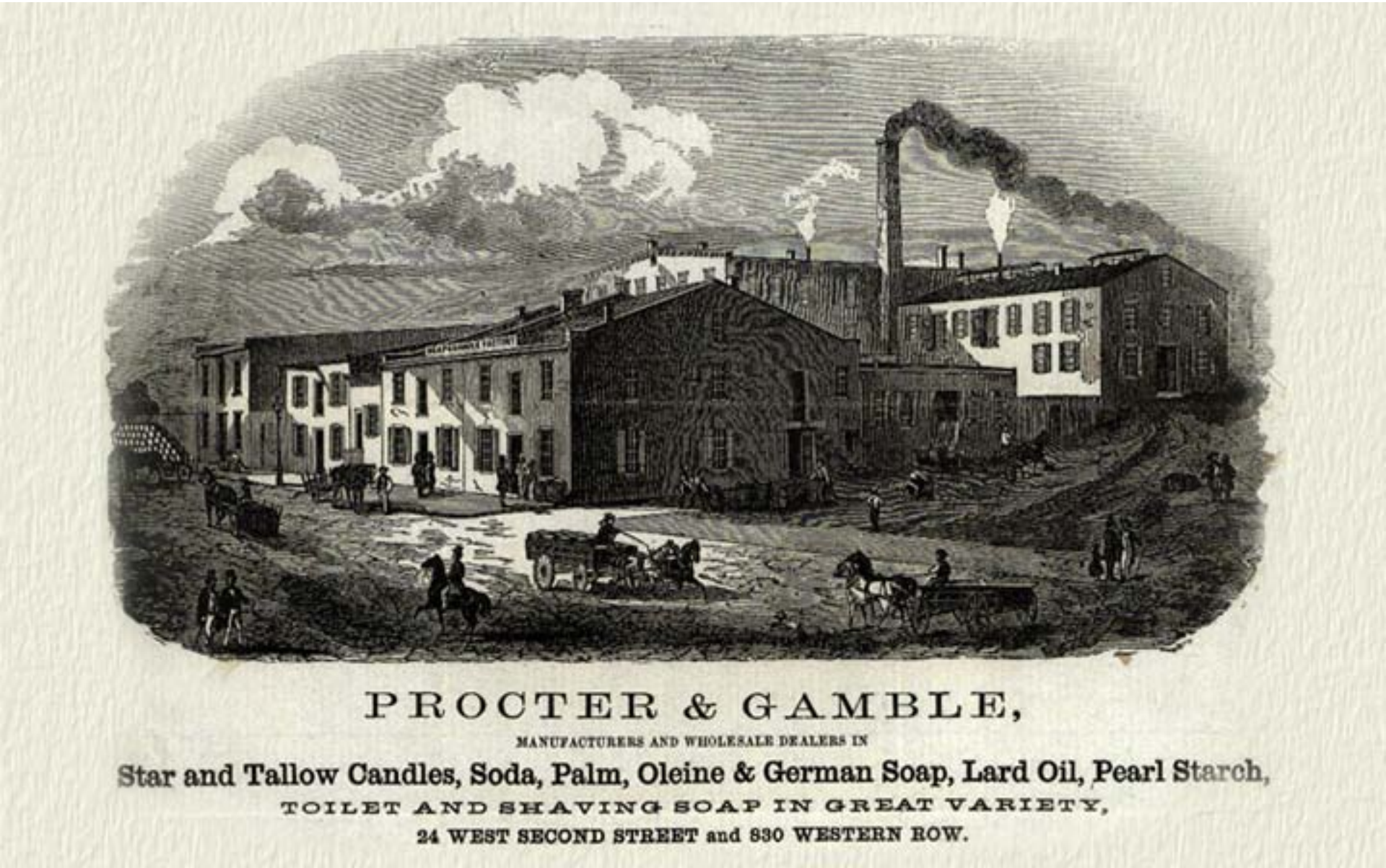
The Amazing Journey of a molecule

Denis O'Sullivan & Antonio Quintieri

Procter & Gamble Company


P&G AT
A GLANCE
Operating in
75
Countries
Serving
4.6
Billion Consumers
Brands sold in
180
Countries

“IT ALL STARTED WITH SOAP & CANDLES”



Serious about innovation

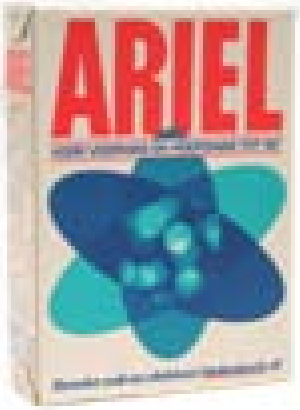
40,000
active patents

8,700
people working in R&D

1,000
PhDs

50 years of excellence at the Ariel Innovation Center in Brussels.

ARIEL
INNOVATION CENTER



1967

1985

1986

1992

2011

2008

2001

1999

1992

Introducing Ariel Pods

Having to receive, store, add, mix, blend, emulsify, fill and ship something like millions of liters of fluids every day, we don't have many choices when it comes to controlling and intensifying our processes

Video removed

Many contradictions at the same time

Increasing flow rates vs. reducing damage to structured fluids;

Shortening residence time vs. high energy;

Faster crystallisation vs. optimising Crystal morphology

Many changes happening at the same time

Viscosity increases while cooling;

Surfactants phases transition as ionic strength decreases;

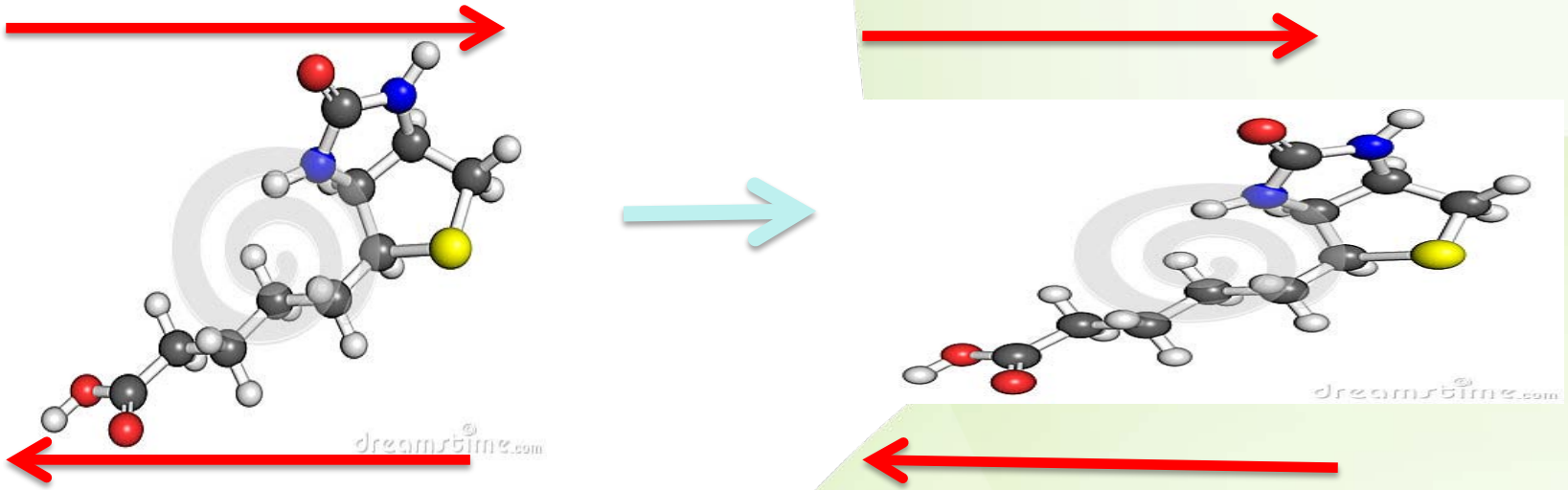
Particles grow while heating;

How to control, measure and intensify all those changes while our molecules travel along our processes ?

Video removed

Back to molecules …

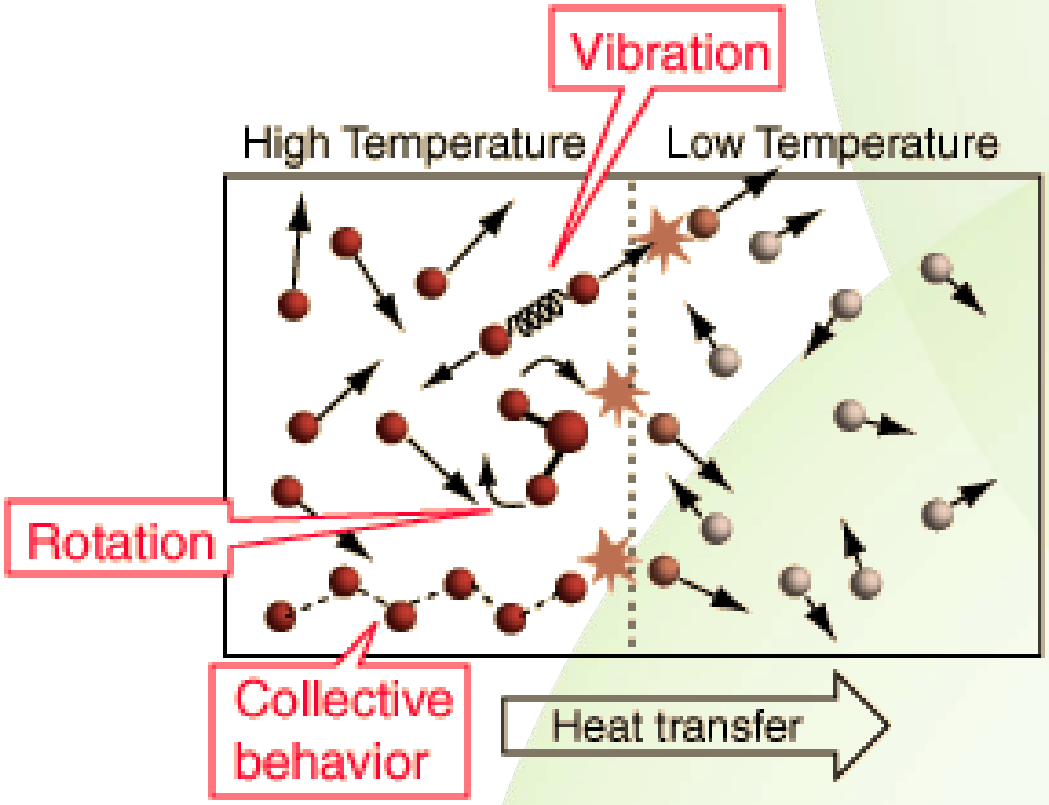
In laminar flow, **shear forces** must be the same at all scales



In turbulent flow, **energy density** a the macroscopic "equivalent" of shear-rate.

In the perfect world …

Temperature and **Temperature Gradients** should also be the same at all scales



In the perfect world …

Also:

- **Residence Times**
- **Concentrations**
- **…**

(you get the idea)

Batch vs. Continuous

Batch vs. Continuous Processes

	Batch (CSTR)	Continuous
IDEAL	Conditions Change with TIME only.	Conditions change with LOCATION
REALITY	Conditions *not* uniform throughout vessel => different molecules experience different histories.	*Not* ideal plug flow with perfect radial transfer => different molecules experience different histories.
RESULT	• Poor Control of Transformations • Multiple Transformations mixed up. • Less intense “average” conditions.	

Why is this a problem?

- Sub-optimal reaction yield.
- Increased variability
  - Increased cost to meet success criteria
- Reduced Quality Assurance.
- Less capacity for Innovation
  - Like innovating in a black box

Why MicroProcessing?

It’s continuous processing without the downsides:

- “Perfect” radial mixing.
- Sequential Transformations
- Controlled Conditions
- Possibility to Intensify

Case-Study : **Crystallisation**

Background

- Efficacy highly morphology-dependent.
- Current Batch Process produces a mix of cylindrical and other morphologies.
- Theoretical model: with “perfect” morphology, could be 3X more effective.

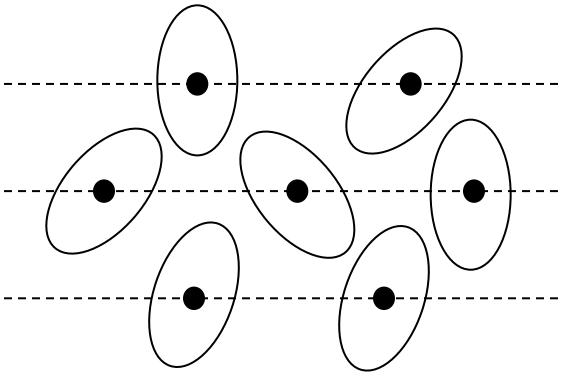
Crystallisation Optimisation

Literature shows three different modes of Crystallisation:

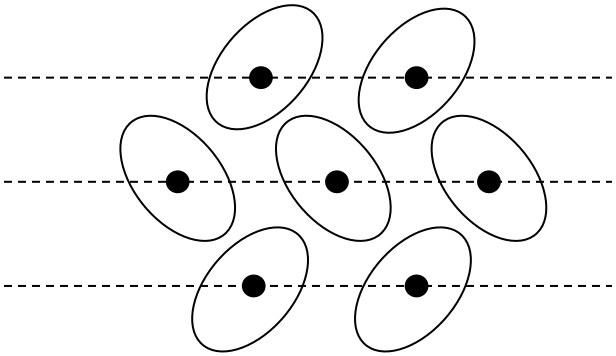
- α-crystals
- β'-crystals
- β-crystals

Cross-Sectional Structures of Triglycerides

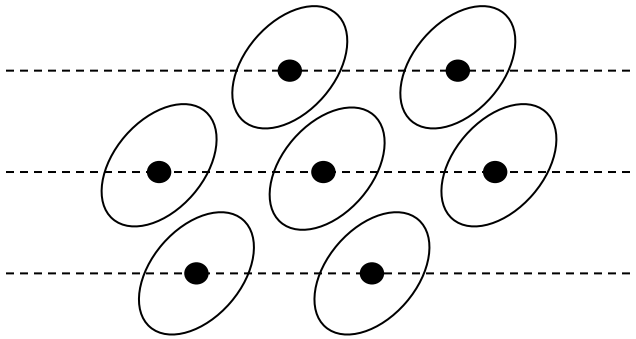
Freedom of molecular motion



Alpha



Beta Prime



Beta

Characteristics of Triglyceride Polymorphs

Alpha	Beta-Prime	Beta
Microscopic Analyses		
Platelet	Fine needle	Long needle
5 μ	1 μ	25-50 μ
Infrared Spectroscopic Analyses		
A singlet at 720 cm^{-1}	A doublet at 719 and 727 cm^{-1}	A singlet at 717 cm^{-1}

The Challenge

- α-crystals – form below 65C
- β'-crystals – form from 60 – 70C
- β-crystals – form from 70 – 75C

We want β-crystals …

The Challenge

… we want β-crystals

… but they have the slowest crystallisation kinetics …

to get a high % of β'-crystals, we need to

keep 75C > T > 70C and

provide continuous gentle shear

The Academic Challenge

How to keep 75C > T > 70C and provide continuous gentle shear ?

In a university lab, you can hold the solution at 73C and stir gently for a month …

The Industrial Challenge

Crystallisation Temperature is 75C!

Nucleation above 70C is far too slow!

… in industry things must happen fast.

The Creative Industrial Solution

Complex, confidential process

Gives increased β-crystals

But still a mix of crystal morphologies.

The microProcessing Solution

Emulsify at very high-energy/high-T.

Shock-cool (2secs) to 40C to nucleate.

Shock-heat immediately to 73C to *stop nucleation, before any crystals have formed*.

Cool with shear at 73C.

.

Result

- *First* trial better than batch.
- Optimisation enabled higher % β-crystals.

And importantly:

- New understanding
  - can improve current process by 50% !!

Why did this work?

- Separated transformations.
- Optimised conditions for each transformation separately.
- Controlled these precisely.
- Intensified mixing, cooling, heating.

microProcessing Today in P&G

- R&D tool, enabling
  - fundamental understanding
  - process optimisation.
- Flowrate too low for production
- Capital reduction not a big opportunity,
  - as most capital is spent on infrastructure.

… but all this may change …

Thank you!!

Questions?