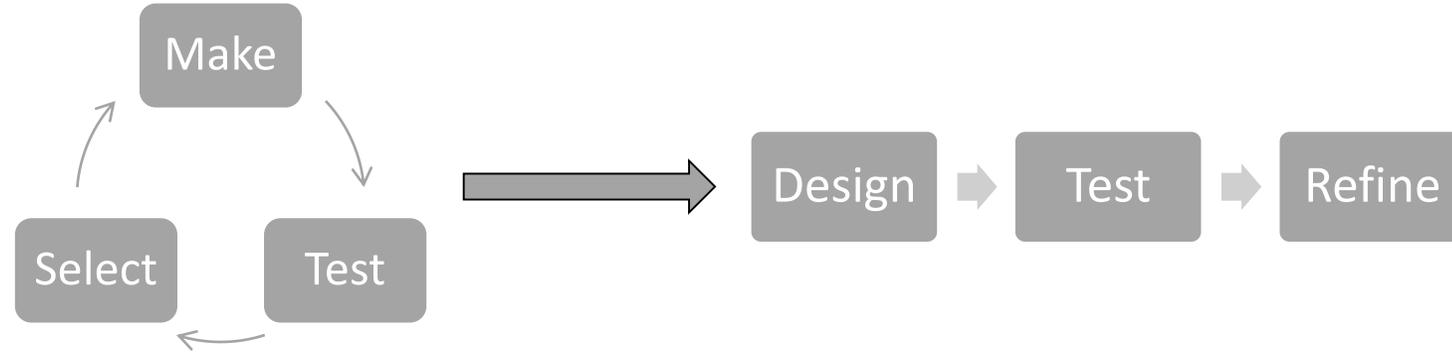ADVANCED DIGITAL DESIGN OF PHARMACEUTICAL THERAPEUTICS

Overview of Industrial Case Studies

Richard Storey (AZ) and Martyn Ticehurst (Pfizer)

Moving towards design

Make → Test → Select (cycle)

Trial and error, making and testing, leading to extensive consumption of material and time.

Risk of correlation driven understanding.

Reduced experiments

Increased understanding

Design → Test → Refine

Predictive design, followed by prototype testing and refinement. The better the prediction, the fewer the prototypes.
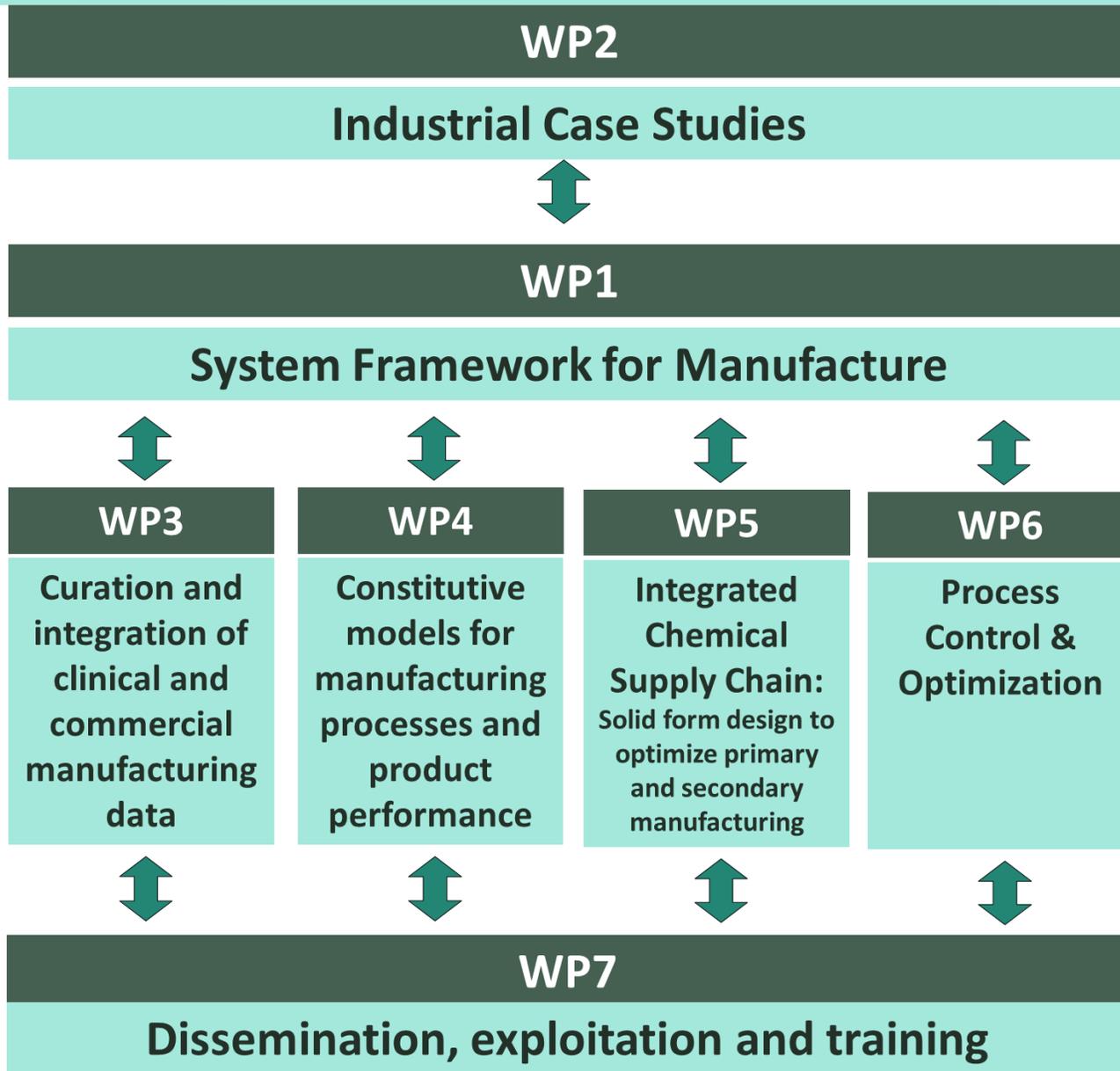
Hypothesis driven understanding.

- Change in culture needed to ensure utilisation of digital design as a *core* part of experimentation
- Case studies have demonstrated how different projects can utilise digital design to aid development

The ADDoPT project has allowed many case studies to be developed to demonstrate the value of digital design in modern development environments

ADD PT

WP2

Industrial Case Studies

WP1

System Framework for Manufacture

WP3	**WP4**	**WP5**	**WP6**
Curation and integration of clinical and commercial manufacturing data	Constitutive models for manufacturing processes and product performance	Integrated Chemical Supply Chain: Solid form design to optimize primary and secondary manufacturing	Process Control & Optimization

WP7

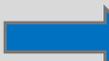**Dissemination, exploitation and training**

Cases studies sit above the main work-engines of ADDoPT (Work packages 1, 3, 4, 5, 6) to:

1. Demonstrate the utilisation of modelling frame-work, data driven models and mechanistic models

2. Drive the specific development of new modelling tools to exemplify the exploitation of digital design approach in solving manufacturing problems

Two way working to ensure models are relevant to industry

ADDoPT

Case Study Heat Map

ADDoPT WP	Primary Manufacturing		Secondary Manufacturing		Performance
	API Crystallis'n & isolation	API milling, flow and feeders	Drug Product, Blending, flow and Granulat'n	Drug Product compression and coating	Product Performance e.g. Dissolution & Stability
1. Systems based approach	PFE5, GSK3	PFE5, GSK3	PFE5, GSK3	PFE5, GSK3	PFE5, GSK3
1. Hybrid models		GSK3			AZ3
3A Lattice energies	PFE6				PFE6
3B Physical props to processing	AZ1	PFE3, CrossPrime1	CrossPrime1	PFE2	
3C Solubility	PFE4				PFE4
4A Solid - state & interfacial props	CrossPrime2 Leeds2	Leeds2	Leeds2	PFE2, Leeds2, CrossPrime2	GSK4, Leeds1, CrossPrime2
4B Crystallisation & isolation	AZ1, GSK1, PFE8, CMAC2			PFE2	
4C Milling & flow		PFE1, AZ4	AZ2		
4D Formulation			AZ2		AZ3
5 Solid form & particle design	PFE4, PFE9, CrossPrime2	PFE9		CrossPrime1	PFE4, CrossPrime2
6 Process optimisation & control	CMAC1		AZ2, PFE7	PFE7	

ADDoPT use only