PhD Advert Template

**Project title: Stoichiometric and kinetic modelling of multiple chemical reactions from laboratory data**

Project ID *(optional)*:

Accept all year-round applications:

Funding information: Self-funded students only

Project description:

The fine chemical and pharmaceutical industries have always focussed on new product development as a means of growth, with time to market being a critical success factor. A major bottleneck in the transition from chemistry research to process development is that more quantitative information, regarding the chemical synthesis, is needed. Within these industries multi-purpose plants which are suitable for a variety of customer specifications are often used. This leads to fast changing discontinuous processes incorporating batch or semi-batch reactors. A major problem facing these companies is the scale up of a process from laboratory to full-scale production in the shortest possible time, preferably avoiding pilot-plant testing. The appropriate use of available laboratory data to facilitate new product development represents a promising industrial opportunity as well as a considerable challenge. Ideally, such quantitative information will be obtained in the early stages where experiments are done on a small scale in relatively cheap flexible equipment rather than in later stages with less flexible and more expensive equipment.

Since any chemical synthesis performed in these industries is usually complex, their reaction mechanisms are normally poorly understood. However, the over-riding concern for process development is not to gain a detailed mechanistic understanding, it is to rapidly develop stoichiometric and kinetic models of the reactions that may be used to perform process optimisation and scale-up studies. Despite earlier efforts the rapid elucidation of both the stoichiometric and kinetic model of a chemical synthesis remains a limiting step requiring considerable time, expertise and intellectual effort. In this work a systematic method for generating all possible chemical reactions and then determining an unambiguous kinetic model of a chemical synthesis will be demonstrated. The developed method will not rely on a detailed mechanistic understanding of a chemical synthesis. However, it will use information that is known about the system, i.e., chemical species involved in the reactions (their molecular weights, atomic structure etc.), species mass balances, and where appropriate heat and mass transfer characteristics etc. to develop stoichiometric and subsequently kinetic descriptions of the chemical reactions taking place between the observed species. The method will be demonstrated using experimental data.

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References (optional):

Application enquires: *Dr Mark J. Willis*

[*https://www.ncl.ac.uk/engineering/staff/profile/markwillis.html*](https://www.ncl.ac.uk/engineering/staff/profile/markwillis.html)

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PhD Disciplines & Subject areas

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[ ]  agricultural sciences

[ ]  agricultural technology

[ ]  arable farming

[ ]  livestock farming

[ ]  forestry & arboriculture

[ ]  other

Anthropology

[ ]  biological anthropology

[ ]  social anthropology

[ ]  other

Architecture, Building & Planning

[ ]  architecture

[ ]  built environment

[ ]  construction management

[ ]  landscape architecture

[ ]  rural planning

[ ]  surveying

[ ]  urban planning

[ ]  other

Biological Sciences

[ ]  bacteriology

[ ]  behavioural biology

[ ]  biochemistry

[ ]  biodiversity

[ ]  bioinformatics

[ ]  biophysics

[ ]  biotechnology

[ ]  cancer biology

[ ]  cell biology

[ ]  developmental biology

[ ]  ecology

[ ]  ecotoxicology

[ ]  entomology

[ ]  environmental biology

[ ]  evolution

[ ]  genetic engineering

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[ ]  human genetics

[ ]  immunology

[ ]  marine biology

[ ]  microbiology

[ ]  molecular biology

[ ]  molecular genetics

[ ]  neuroscience

[ ]  parasitology

[ ]  plant biology

[ ]  plant cell biology

[ ]  reproductive biology

[ ]  structural biology

[ ]  systematic biology

[ ]  virology

[ ]  zoology

[ ]  other

Business & Management

[ ]  accounting

[ ]  business

[ ]  e business

[ ]  education management

[ ]  event management

[ ]  hospitality

[ ]  human resource management

[ ]  management

[ ]  marketing

[ ]  project management

[ ]  sport management

[ ]  tourism

[ ]  other

Chemistry

[ ]  analytical chemistry

[ ]  applied chemistry

[ ]  computational chemistry

[ ]  environmental chemistry

[ ]  industrial chemistry

[ ]  inorganic chemistry

[ ]  organic chemistry

[ ]  petrochemical chemistry

[ ]  pharmaceutical chemistry

[ ]  physical chemistry

[ ]  polymer chemistry

[ ]  structural chemistry

[ ]  synthetic chemistry

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Communication & Media Studies

[ ]  broadcast media

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[ ]  journalism

[ ]  print media

[ ]  production

[ ]  public relations

[ ]  publishing

[ ]  other

Computer Science

[ ]  artificial intelligence

[ ]  computer architectures

[ ]  computer vision

[ ]  computer graphics

[ ]  cyber security

[ ]  data science

[ ]  human computer interaction

[ ]  internet of things

[ ]  machine learning

[ ]  networks

[ ]  quantum computing

[ ]  software engineering

[ ]  videogames

[ ]  other

Creative Arts & Design

[ ]  animation

[ ]  art

[ ]  crafts

[ ]  creative writing

[ ]  dance

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[ ]  drama

[ ]  fashion

[ ]  film studies

[ ]  fine art

[ ]  graphic design

[ ]  interior design

[ ]  music

[ ]  music technology

[ ]  photography

[ ]  theatre studies

[ ]  other

Economics

[ ]  econometrics

[ ]  financial economics

[ ]  macroeconomics

[ ]  microeconomics

[ ]  political economics

[ ]  other

Education

[ ]  further education

[ ]  higher education

[ ]  nursery education

[ ]  primary education

[ ]  secondary education

[ ]  special needs education

[ ]  other

Engineering

[ ]  acoustics engineering

[ ]  aerospace engineering

[ ]  atomic engineering

[ ]  automotive engineering

[ ]  bioengineering

[ ]  biomedical engineering

[x]  chemical engineering

[ ]  civil engineering

[ ]  communications engineering

[ ]  control systems

[ ]  cybernetics

[ ]  dynamics

[ ]  electrical engineering

[ ]  electronic engineering

[ ]  energy technologies

[ ]  environmental engineering

[ ]  fluid mechanics

[ ]  gas engineering

[ ]  geotechnical engineering

[ ]  integrated engineering

[ ]  manufacturing engineering

[ ]  marine engineering

[ ]  mechanical engineering

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[ ]  mechatronics

[ ]  nanotechnology

[ ]  offshore engineering

[ ]  petroleum engineering

[ ]  robotics

[ ]  solid mechanics

[ ]  structural engineering

[ ]  structural mechanics

[x]  systems engineering

[ ]  thermodynamics

[ ]  other

Environmental Sciences

[ ]  climate science

[ ]  hydrology

[ ]  marine sciences

[ ]  meteorology

[ ]  pollution

[ ]  soil science

[ ]  other

Finance

[ ]  actuarial science

[ ]  banking

[ ]  financial management

[ ]  insurance

[ ]  investment

[ ]  taxation

[ ]  other

Food Sciences

[ ]  food hygiene

[ ]  food production

[ ]  other

Forensic and Archaeological Sciences

[ ]  archaeological science

[ ]  forensic science

[ ]  other

Geography

[ ]  agricultural geography

[ ]  cultural geography

[ ]  economic geography

[ ]  environmental geography

[ ]  geographical information systems gis

[ ]  historical geography

[ ]  human geography

[ ]  marine geography

[ ]  physical geography

[ ]  political geography

[ ]  remote sensing

[ ]  social geography

[ ]  transport geography

[ ]  urban geography

[ ]  other

Geology

[ ]  applied geology

[ ]  geochemistry

[ ]  geophysics

[ ]  geoscience

[ ]  geotechnology

[ ]  hydrogeology

[ ]  marine geology

[ ]  palaeontology

[ ]  seismology

[ ]  volcanology

[ ]  other

History & Archaeology

[ ]  african history

[ ]  american history

[ ]  ancient history

[ ]  archaeology

[ ]  asian history

[ ]  australasian history

[ ]  british and irish history

[ ]  economic history

[ ]  european history

[ ]  heritage studies

[ ]  history

[ ]  history of art

[ ]  history of religions

[ ]  history of science

[ ]  medieval history

[ ]  military history

[ ]  modern history

[ ]  russian history

[ ]  social history

[ ]  world history

[ ]  other

Information Services

[ ]  information security

[ ]  information systems

[ ]  librarianship

[ ]  other

Languages, Literature & Culture

[ ]  african studies

[ ]  american studies

[ ]  asian studies

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[ ]  english language

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[ ]  other

Law

[ ]  criminal law

[ ]  commercial law

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Linguistics & Classics

[ ]  ancient greek

[ ]  celtic studies

[ ]  classics

[ ]  latin

[ ]  linguistics

[ ]  other

Materials Science

[ ]  ceramics

[ ]  glass

[ ]  metallurgy

[ ]  polymers

[ ]  textiles

[ ]  other

Mathematics

[ ]  applied mathematics

[ ]  applied statistics

[ ]  computational mathematics

[x]  data analysis

[ ]  engineering mathematics

[ ]  mathematical modelling

[ ]  medical statistics

[ ]  operational research

[ ]  probability

[ ]  pure mathematics

[ ]  statistics

[ ]  stochastic processes

[ ]  other

Medicine

[ ]  anatomy

[ ]  audiology

[ ]  biomechanics

[ ]  cardiology

[ ]  complementary medicine

[ ]  dentistry

[ ]  endocrinology

[ ]  epidemiology

[ ]  neural engineering

[ ]  neurology

[ ]  nutrition

[ ]  ophthalmology

[ ]  optometry

[ ]  pathology

[ ]  pharmacology

[ ]  pharmacy

[ ]  physiology

[ ]  physiotherapy

[ ]  podiatry

[ ]  radiology

[ ]  speech science

[ ]  tissue engineering

[ ]  toxicology

[ ]  other

Nursing & Health

[ ]  adult nursing

[ ]  community nursing

[ ]  counselling

[ ]  dental nursing

[ ]  environmental health

[ ]  health informatics

[ ]  medical nursing

[ ]  mental health nursing

[ ]  midwifery

[ ]  occupational health

[ ]  occupational therapy

[ ]  paediatric nursing

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[ ]  surgical nursing

[ ]  other

Philosophy

[ ]  ethics

[ ]  metaphysics

[ ]  philosophy of science

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Physics

[ ]  acoustics

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[ ]  chemical physics

[ ]  computational physics

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[ ]  experimental physics

[ ]  medical physics

[ ]  nuclear physics

[ ]  optical physics

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Politics & Government

[ ]  development studies

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Psychology

[ ]  child psychology

[ ]  clinical psychology

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Sociology

[ ]  criminology

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[ ]  gender studies

[ ]  socio economics

[ ]  social work

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Sport & Exercise Science

[ ]  sport coaching

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[ ]  sport performance

[ ]  sport technology

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Theology & Religious Studies

[ ]  divinity

[ ]  religious studies

[ ]  theology

[ ]  other

Veterinary Sciences

[ ]  animal welfare

[ ]  veterinary dentistry

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[ ]  veterinary nursing

[ ]  veterinary nutrition

[ ]  veterinary pathology

[ ]  other