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*](mailto:mark.willis@ncl.ac.uk)

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

**We will also need to link your PhD advert up to the subject keywords below so that your PhD studentship can be found on findaphd.com. Please highlight up to three relevant keywords from the lists provided below.**

**FindaPhD.com**  
You can select up to **10 subject areas**.

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

genetics

genomics

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

other

Communication & Media Studies

broadcast media

digital media

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

design

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

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

mechanics

mechatronics

nanotechnology

offshore engineering

petroleum engineering

robotics

solid mechanics

structural engineering

structural mechanics

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

australasian studies

chinese

danish

dutch

english language

english literature

european studies

finnish

french

german

italian

japanese

middle eastern studies

norwegian

portuguese

russian

spanish

swedish

other

Law

criminal law

commercial law

contract law

property law

other

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

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

paramedical science

surgical nursing

other

Philosophy

ethics

metaphysics

philosophy of science

other

Physics

acoustics

astronomy

astrophysics

chemical physics

computational physics

electromagnetism

environmental physics

experimental physics

medical physics

nuclear physics

optical physics

particle physics

quantum mechanics

solid state physics

space science

theoretical physics

other

Politics & Government

development studies

government

international relations

politics

public policy

other

Psychology

child psychology

clinical psychology

community psychology

counselling psychology

developmental psychology

educational psychology

forensic psychology

health psychology

neuropsychology

occupational psychology

organisational psychology

psychotherapy

sport psychology

other

Sociology

criminology

disability studies

gender studies

socio economics

social work

other

Sport & Exercise Science

sport coaching

sport development

sport performance

sport technology

sport therapy

other

Theology & Religious Studies

divinity

religious studies

theology

other

Veterinary Sciences

animal welfare

veterinary dentistry

veterinary medicine

veterinary nursing

veterinary nutrition

veterinary pathology

other