Optimised Small Scale Reactor Technology, a new approach for the Australian Biodiesel Industry

The application of Computational Fluid Dynamic (CFD) Modelling techniques to homogeneous catalysed methanolysis reactors

This thesis is presented for the degree of Doctor of Philosophy in Engineering

By

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B.E. (Renewable Energy Engineering and Instrumentation & Control Engineering) 2007

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2010

DECLARATION

I declare that this thesis is my own account of my research and contains, as its main content, work which has not previously been submitted for a degree at any tertiary education Institution.

…………………………….

Karne de Boer

ABSTRACT

With growing concern over peak oil and global warming many are urgently seeking alternatives to petro-diesel to fuel growing economies. Biodiesel, a diesel equivalent derived from vegetable oils and animal fat, is one such alternative. Large scale uptake of biodiesel, however, is limited by the availability of low cost, sustainable feedstocks.

In the context of feedstock limitations in Australia, this thesis examines the complete biodiesel system from feedstock to end consumer via production technology. The result of this investigation was the identification of integrated small scale biodiesel production (less than 5 million L/yr) as an economically viable niche for the Australian biodiesel industry. This is especially the case in remote locations.

To this end, a new production model, based upon small scale operations in regional industry hubs, was presented and validated with a case study in South Western Australia. This production model presents a new approach for the Australian biodiesel industry.

Having established the economic sustainability of the small scale production model, this work lays a foundation for its technical viability by optimising the reactor technology at the heart of biodiesel production. The following two questions are examined in the pursuit of reactor technology optimisation for small scale production:

- What is the most suitable catalyst for small scale production?
- Can an accurate model of the reactor be developed to facilitate optimisation?

The first question necessitated a detailed review of biodiesel production technology. The fruit of this review was the identification of homogeneous catalysed technology as the most suitable method for small scale biodiesel production. The second question required a reactor model that could determine the level of conversion on the basis of reactor temperature and residence time (flow-rate).

Further investigation into the homogeneous catalysed reaction medium suggested a two part model, with the first focusing on flow characteristics to maintain dispersion of the reacting phases, and the second on kinetics to determine conversion. Due to the multiphase nature of the reaction medium, the first part was developed as a Computational Fluid Dynamic (CFD) model of the flow through Bluediesel PTY LTD's tubular reactor in ANSYS CFX. This model drew heavily on literature in the field of oil and water flows and was verified with flow visualization studies of the reactor. The second part of the model was built in MATLAB on the basis of biodiesel kinetic studies and was verified with data from Bluediesel PTY LTD's plant.

This model was ran at a number of operating conditions and configurations to determine the minimum total cost of a small scale reactor while maintaining suitable levels of conversion. This optimisation work represents the first application of CFD modelling to a biodiesel reactor and can be used as a basis for further work in this area.

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PUBLICATIONS

de Boer, K., Bahri, P. A. (2009). *Forging Ahead with Small Scale Production: A different Approach for the Australian Biodiesel Industry in Difficult Times*. Paper presented at the Bioenergy Australia 2009 conference, Radisson Resort Gold Coast Queensland, Australia, 8th-10th December.

de Boer, K., Bahri, P. A. (2009). *Investigation of Liquid-Liquid Two Phase Flow in Biodiesel Production*. Paper presented at the Seventh International Conference on Computational Fluid Dynamics in the Minerals and Process Industries, Rydges Hotel, Melbourne, Australia, 9th -11th December.

De Boer, K., Bahri, P.A. (2010). Supercritical Methanol for fatty acid methyl ester production: A Review, ,Biomass and Bioenergy (2010), doi:10.1016/j.biombioe.2010.11.037

ACKNOWLEDGEMENTS

As this doctoral journey has comes to a close I am provided with an opportunity to stop at a unique vantage point and survey the road that has been traversed. First and foremost I must praise my Lord, Creator and Saviour Jesus Christ who gave me breath to breathe and a brain to use. I did this work so that I could become a better engineer and serve Him better by helping others throughout this world and he has enabled me to finish it.

I want to thank my dad Robbie, mum Annie and brother Shaun who have supported me throughout seven years of university. Special thanks are due to my dad who was my constant companion over the last three years and he will be as happy as I am to see this thesis submitted. Without his support, provision of clean clothes, food and encouragement I don't think I would be here now.

I can do nothing but thank my Supervisor, friend and colleague Professor Parisa A. Bahri who has constantly supported me in this work and has demonstrated a professionalism and kindness beyond what is required. Parisa is an amazing, dedicated and talented woman who I have the deepest respect for, in fact if it wasn't for her persistence and foresight I would never have done a PhD in the first place. I also thank her administrative assistants Roselina Stone and Bronwyn Phua who were a great help. I thank Murdoch University for the provision of this canditure and this opportunity as well as the Australian Governement for the provision of a scholarship

I am indebted to my friends and roommates at University especially Jan, Aresh, Sorousha, Shabnam, Mehdi and Mark who have made this journey interesting while also giving it a very strong Iranian flavor. I also am very thankful to Bluediesel PTY LTD for their scholarship support and access to their commercial plant. I very much thank Andrew and the board of directors for giving me this chance and Richard for helping me out at any opportunity.

Finally, I want to thank my beautiful wife Pamela, who I met and married in the final year of my canditure, she carried my dad's vision for me finishing this work and is a great source of joy as my constant companion.

NOMENCLATURE

ACRONYMS

ARF – Australian Renewable Fuels

ASAE (now ASABE) - American Society of Agricultural and Biological Engineers

ASP – Aquatic Species Program

AQIS – Australian Quarantine and Inspection Service

BAA – Biofuels Association of Australia

BDI – BioDiesel International

BIA – Biodiesel Industries Australia

BPL – Biodiesel Producers Limited

CFD – Computational Fluid Dynamics

CFPP – Cold Filter Plugging Point

CNG – Compressed Natural Gas

CO_2-e/km – Grams of CO_2 per km

CSTR – Continuous Stirred Tank Reactor

DOE – Department of Energy

EJ – Exajoule

FAME – Fatty Acid Methyl Ester

FFA – Free Fatty Acid

GUI – Graphical User Interface

GUIDE – Graphical User Interface Development Environment

IPCC – Intergovernmental Panel on Climate Change

LCA – Life Cycle Analysis

LPG – Liquid Petroleum Gas

MTOE – Metric Tonne of Oil Equivalent

MBPD - Million Barrels Per Day (1 barrel = 159 L)

NREL - National Renewable Energy Laboratory

ODE – Ordinary Differential Equation

OECD - Organisation for Economic Co-operation and Development

OEM – Original Equipment Manufacturer

OPEC – Organisation of Petroleum Exporting Countries

PBR – Photo Bio- Reactor

PFR – Plug Flow Reactor

PPV – Polar Phase Volume fraction

REACT – Renewable Energy ACTion

RIRDC – Rural Industries Research and Development Commission

UCO – Used Cooking Oil

ULSD – Ultra Low Sulphur Diesel

USA – United States of America

THF – Tetra-Hydro-Furan

TWh – Terra Watt hour

VARIABLES

E	Specific energy	J
i	internal energy	J
k	Thermal conductivity	W/mK
L	Characteristic length scales	m
p	Pressure	kg/ms^2 or Pa
S_{xx}	Source term	
t	Time	s
T	Temperature	°C or °K
u	Velocity vector	m/s
U	Characteristic velocity	m/s
U	Mean velocity vector	m/s
u,v,w	x,y,z-component of the velocity	m/s
x,y,z	Cartesian Coordinates	m

GREEK SYMBOLS

κ	Turbulent kinetic energy	J/kg
ρ	Density	kg/m^3
μ	Dynamic viscosity	kg/ms
Φ	Dissipation function	kg/ms^3
Γ	Diffusion coefficient	m^2/s
ν	Kinematic viscosity	stokes = 0.0001 m^2/s
ϕ	General variable	

SUB/SUPER INDEX

x,y,z	Direction
wt-oil	Weight of oil
c	Continuous
d	Dispersed
m	Mixture