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SIMULATION OF COMPLEX MULTI-PHASE, MULTI-COMPONENT, REACTING FLOWS IN POROUS MEDIA

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Abstract

In this study we are concerned with the modelling of multi-component, multiphase chemically reacting flows in porous media, with particular application to the spontaneous combustion of coal and the extraction of coalbed methane.

These two related problems involve complex multiphase, multi-component flow in a porous medium. Chemical reactions, adsorption, gaseous diffusion and changes in porosity and permeability are important in one or both of these problems. These matters are discussed in general in the first few chapters of the thesis.

Several models for the spontaneous combustion of coal that include the effect of a diminishing reaction rate are investigated and a new formulation in the form of a generic power law model is introduced.

A numerical module for modelling the spontaneous combustion of coal is described, based on the TOUGH2 code. A new equation of state (EOS) module is developed including realistic physical properties for all gases involved. The modified version of TOUGH2 is used for modelling the adiabatic method for testing the reactivity of coal samples. The results agree very well with experimental measurements for coal samples from different mines in New Zealand and Australia.

Moisture effect on the reaction rate was then introduced to TOUGH2 using a new two-phase EOS module with water and air broken into its main components (Nitrogen, Oxygen, Carbon dioxide and Argon).

Finally the production of methane from low rank coalbeds is investigated. A new EOS for mixture of water and methane is developed and incorporated into the TOUGH2 code to produce a new and versatile coalbed methane simulator. It is validated by running
some simple test problems and comparing results with those obtained with the commercial COMET simulator.
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To My Homeland Iraq
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Because of the extensive literature review and the many different applications discussed in this work, it is impossible to have a common notation throughout the thesis. The nomenclature given below includes the notation used throughout the work, while the other notation is defined differently as it appears in each chapter.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Area</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$A_0$</td>
<td>Arrhenius pre-exponential factor (first order)</td>
<td>$1/s$</td>
</tr>
<tr>
<td>$A_1'$</td>
<td>Arrhenius pre-exponential factor for coal (Chapter 6)</td>
<td>$m^3/kg_{coal} s$</td>
</tr>
<tr>
<td>$A_0''$</td>
<td>Arrhenius pre-exponential factor (zero order)</td>
<td>$1/s$</td>
</tr>
<tr>
<td>$Bi$</td>
<td>Biot number $Bi = hx/K$</td>
<td></td>
</tr>
<tr>
<td>$C$</td>
<td>Concentration</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific heat capacity</td>
<td>$kJ/kgK$</td>
</tr>
<tr>
<td>$c_K$</td>
<td>Cozeny’s constant</td>
<td></td>
</tr>
<tr>
<td>$c$</td>
<td>Compressibility</td>
<td>$1/Pa$</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
<td>$m^2/s$</td>
</tr>
<tr>
<td>$D_{th}$</td>
<td>Thermal diffusivity $D_{th} = K/\rho C_p$</td>
<td>$m^2/s$</td>
</tr>
<tr>
<td>$d_\beta^{(\kappa)}$</td>
<td>Diffusion coefficient of phase $\beta$ in component $\kappa$</td>
<td>$m^2/s$</td>
</tr>
<tr>
<td>$d$</td>
<td>Diameter</td>
<td>$m$</td>
</tr>
<tr>
<td>$E_a$</td>
<td>Activation energy</td>
<td>$J/mol$</td>
</tr>
<tr>
<td>$F_f$</td>
<td>Formation factor (Chapter 3)</td>
<td></td>
</tr>
<tr>
<td>$F^{(\kappa)}$</td>
<td>Flux of component $\kappa$</td>
<td>$kg/m^2s$ or $J/m^2s$</td>
</tr>
<tr>
<td>$f^{(\kappa)}$</td>
<td>Mass fraction of component $\kappa$ adsorbed per mass of solid</td>
<td>$kg^{\kappa}/kg^{solid}$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td></td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
<td>$m/s^2$</td>
</tr>
<tr>
<td>$G_s^{(i)}$</td>
<td>Gas storage capacity of component $i$</td>
<td>$m^3/kg_{coal}$</td>
</tr>
<tr>
<td>$h$</td>
<td>Heat transfer coefficient (convection)</td>
<td>$W/m^2K$</td>
</tr>
<tr>
<td>$h$</td>
<td>Cleat thickness (Chapter 8)</td>
<td>$m$</td>
</tr>
<tr>
<td>$H^{(\kappa)}$</td>
<td>Enthalpy of component $\kappa$</td>
<td>$J/kg$</td>
</tr>
<tr>
<td>$h_{fg}$</td>
<td>Latent heat of water</td>
<td>$J/kg$</td>
</tr>
<tr>
<td>$J$</td>
<td>Jacobian matrix</td>
<td></td>
</tr>
<tr>
<td>$K$</td>
<td>Thermal conductivity</td>
<td>$W/mK$</td>
</tr>
<tr>
<td>$k$</td>
<td>Permeability</td>
<td>$m^2 (10^{-12} \text{ Darcy})$</td>
</tr>
<tr>
<td>$K_d$</td>
<td>Distribution coefficient</td>
<td>$m^3/kg_{solid}$</td>
</tr>
<tr>
<td>$K_h$</td>
<td>Henry’s constant</td>
<td>$Pa (N/m^2)$</td>
</tr>
<tr>
<td>$L$</td>
<td>Length</td>
<td>$m$</td>
</tr>
<tr>
<td>$L_e$</td>
<td>Effective length</td>
<td>$m$</td>
</tr>
<tr>
<td>$M_{\beta}^{(\kappa)}$</td>
<td>Mass accumulation term of component $\kappa$ in phase $\beta$</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$M^{NK+1}$</td>
<td>Heat accumulation term in multi-phase system</td>
<td>$J/m^3$</td>
</tr>
<tr>
<td>$MAD$</td>
<td>Adsorbed mass accumulation term</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$MW^{(\kappa)}$</td>
<td>Molar weight of component $\kappa$</td>
<td>$kg/kmol$</td>
</tr>
<tr>
<td>$n$</td>
<td>Reaction order</td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>Unit normal vector</td>
<td></td>
</tr>
<tr>
<td>$NK$</td>
<td>Number of mass components</td>
<td></td>
</tr>
<tr>
<td>$NPH$</td>
<td>Number of phases</td>
<td></td>
</tr>
<tr>
<td>$O_{ad}$</td>
<td>Oxygen adsorbed on the coal surface</td>
<td>$kg_{O_2}/kg_{coal}$</td>
</tr>
<tr>
<td>$P^{(\kappa)}$</td>
<td>Partial pressure of component $\kappa$</td>
<td>$Pa (N/m^2)$</td>
</tr>
<tr>
<td>$P$</td>
<td>Pressure</td>
<td>$Pa (N/m^2)$</td>
</tr>
<tr>
<td>$Q$</td>
<td>Ionic activity product (Chapter 1)</td>
<td></td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat released by reaction (Exothermicity)</td>
<td>$J/kg$</td>
</tr>
</tbody>
</table>
Nomenclature

\( q^{(\kappa)} \)  External sink/source of component \( \kappa \)  \( \text{kg} / \text{m}^3 \text{ s} \) or \( J / \text{m}^3 \text{ s} \)

\( R \)  The universal gas constant (8.3145) \( \text{kJ} / \text{kmol} \text{ K} \)

\( R_t \)  Retardation factor (Chapter 4 and Chapter 8)

\( R_f \)  Recovery factor (Chapter 8)

\( R_{70} \)  Self-heating rate index (40 to 70 °C) (Chapter 6) \( ^\circ \text{C} / \text{hour} \)

\( RH \)  Relative Humidity

\( r \)  Radius \( m \)

\( r^{(\kappa)} \)  Reaction rate of component \( \kappa \) \( \text{kg} / \text{m}^3 \text{ s} \)

\( \text{Re} \)  Reynolds number

\( S \)  Saturation

\( SR \)  Stiffness ratio

\( T \)  Temperature \( ^\circ \text{C} \)

\( T_K \)  Absolute Temperature \( K \)

\( t \)  Time \( s \text{ (sec)} \)

\( t_{pr} \)  Prior reaction (oxidation) time (Chapter 5) \( s \text{ (sec)} \)

\( U \)  The intrinsic velocity \( m / \text{s} \)

\( u \)  Specific internal energy \( J / \text{kg} \)

\( V \)  Darcy’s velocity (volume flux) (\( V = \phi U \)) \( m / \text{s} \)

\( V_n \)  Volume of grid element \( n \) \( m^3 \)

\( X^{(\kappa)}_{\beta} \)  Mass fraction of component \( \kappa \) in phase \( \beta \) \( \text{kg}^{(\kappa)}_{\beta} / \text{kg}^{(\text{total})}_{\beta} \)

\( x \)  Distance \( m \)

\( Z^{(\kappa)} \)  Compressibility factor of component \( \kappa \)

\( \Gamma_n \)  Surface area of grid element \( n \) \( m^2 \)

\( \Gamma \)  Gama function (Chapter 5)

\( \alpha \)  Molar weight ratio

\( \alpha \)  Empirical constant for the diminishing rate law (Chapter 5)

\( \alpha_L \)  Longitudinal dispersion coefficient \( m^2 / \text{s} \)
Nomenclature

\( \alpha_T \) Transverse dispersion coefficient \( m^2/s \)

\( \nabla \) Gradient

\( \lambda \) Reaction rate coefficient

\( \lambda \) Non-isothermal reaction rate coefficient, \( \lambda = A_0 \exp(-E_a/RT) \)

\( \lambda_0 \) Isothermal reaction rate coefficient, \( \lambda_0 = A_0 \exp(-E_a/RT_0) \) (Chapter 5)

\( \rho \) Density \( kg/m^3 \)

\( \nu \) Kinematic viscosity \( \mu/\rho \) \( m^2/s \)

\( \mu \) Dynamic viscosity \( N s/m^2 \ (Pa \ s) \)

\( \mu \) Constant, \( \mu = 1/\delta_0 (1 + \beta) \) (Chapter 5)

\( \nu \) Reaction stoichiometric coefficient

\( \chi \) Mole fraction

\( \beta \) Constant \( \beta = Q/\rho C_p \) (Chapter 4)

\( \beta \) New empirical constant for the diminishing rate law (Chapter 5)

\( \delta_0 \) Modified Frank-Kamenetskii parameter (Chapter 5)

\[ \delta_0 = \left( \frac{E_a}{RT_0^2} \right) (QO_0 A_0 \tau / C_p) \exp \left( \frac{E_a}{RT_0} \right) \]

\( \varepsilon \) Reduced ambient temperature, \( \varepsilon = RT_0/E_a \) (Chapter 5)

\( \gamma \) Incomplete Gamma function (Chapter 5)

\( \zeta \) Constant, \( \zeta = 1/\nu (1 + b) \) (Chapter 5)

\( \nu \) Constant, \( \nu = \sigma/\varepsilon \) (Chapter 5)

\( \theta \) Reduced excess temperature, \( \theta = \left( T - T_0 \right) E_a / R T_0^2 \) (Chapter 5)

\( \sigma \) Constant, \( \sigma = QO_0 / C_p T_0 \) (Chapter 5)

\( \tau \) Tortuosity \( \tau = L_c / L \) \( \tau > 1 \)

\( \tau \) Characteristic time scale \( \left( \tau = t/t_{pr} \right) \) (Chapter 5)

\( \tau \) Sorption time (Chapter 8) \( s \ (sec) \)

\( \tau_f \) Tortuosity factor \( \left( \tau_f = \tau^2 \right) \)

\( \phi \) Porosity
**Nomenclature**

**Subscripts**
- $ad$ Adsorption
- $b$ Bulk
- $coal$ Coal
- $eff$ Effective
- $eq$ Equilibrium
- $f$ Fluid
- $f$ Fracture (Chapter 8)
- $g$ Gas
- $in$ Insoluble mineral (Chapter 2)
- $\circ$ Initial state (initial condition)
- $L$ Langmuir
- $l$ Liquid
- $m$ Mixture
- $m$ Soluble mineral (Chapter 2)
- $m$ Matrix (Chapter 8)
- $p$ Particle
- $r$ Relative
- $s$ Solid
- $s$ Skin (Chapter 8)
- $std$ Standard conditions (101325 Pa and 288.6 K) (Chapter 8)
- $v$ Vapor
- $\beta$ Phase (gas or liquid)

**Superscript**
- $adv$ Advective
- $air$ Air
- $Ar$ Argon
- $CH_4$ Methane
- $CO_2$ Carbon dioxide
Nomenclature

dis  Diffusive (dispersive)
e    Equilibrium
$N_2$  Nitrogen
$O_2$  Oxygen
$sat$  Saturation conditions
$\kappa$  Component (mass or heat)
*  Non-dimensional form (Chapter5)

Abbreviations

BHP  Bottom hole pressure
CBM  Coalbed methane
DEA  differential-algebraic equations
ECBM Enhanced coalbed methane
EOS  Equation of state
FHZ  Fastest heating zone
IFDM  Integrated finite difference method
MINC  Multiple interacting continua
NR  Newton-Raphson
ODE  Ordinary differential equation
PDE  Partial-differential equations
REV  Representative elementary volume
STP  Standard temperature and pressure (101325 $Pa$ and 288.6 $K$)
TDS  Total dissolved solids