Modelling of coal particle transport mechanics in the partially filled screw reactor

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Abstract

Based on the balance equations of mass and momentum, flow behaviour of Newtonian and power-law fluid types have been investigated for the single screw reactor. For this purpose, the helical channel of the screw has been transformed into a cuboids' geometry and the two-dimensional velocity distributions have been calculated steady state using commercial CFD-Code Phoenics™. In favour of good convergence of the mathematical solution, a structured, strictly orthogonal grid has been used. Variable filling degrees have been taken into account by adapting the height of the 'unwrapped' channel. To predict transportation of granular bed, slipping boundary conditions on screw's surface have been used to model momentum flux due to Coulomb's friction.

Keywords
modelling; carbonisation; pyrolysis; screw reactor; granular bed

INTRODUCTION

Iron ore reduction is largely carried out in the blast furnace process which relies on the input of coke. Due to shortness of coking coals, expensive upgrading in the cokery and political conditions to lower emission of carbon dioxide (CO_2), several alternative processes based on smelting reduction and direct reduction are under way. In scope of the European Ultra-Low CO_2 Steelmaking project (ULCOS), a continuous ore reducing process is being developed. This process incorporates partial pyrolysis of non-coking coals in a twin screw reactor type prior being fed into an ore smelting cyclone as a fuel and reducing agent. Direct reduction in a mixed iron-coal smelting bath is expected to lower specific coal requirement by 25% in comparison to common blast furnace processes. The purpose of the screw reactor is to preheat and upgrade the feed coals by partial pyrolysis, *i.e.* to increase the specific carbon fraction by lowering specific hydrogen and oxygen fractions, while heating the reactor by combustion of the pyrolysis gases. In order to determine preferable geometric layouts and working conditions of the screw reactor, occurring transport phenomena are investigated with by means of a mathematical model.

Up to present, an isothermal single screw reactor model is available for prediction of velocity distributions for incompressible flow in the screw channel. The fully developed model will include chemical reaction of the coals initiated by local temperature and partial pressure of coal species. As the temperature field of the indirectly heated reactor primarily depends on effective thermal conductivity and heat capacity of granular bed, knowledge of local shear rate is important since it affects the effective thermal conductivity.

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MATHEMATIC MODELLING

Fig. 1 shows a cross section of the single screw reactor. For equal pressure at inlet and outlet, flow in the helical processing domain is caused only by relative movement between screw and surrounding barrel, *i.e.* rotation of the screw while keeping the barrel fixed. Flow is a result of momentum flux at the interfaces between the reactor and fluid. Two transport mechanics have been considered:

Case 1: The fluid adheres (non-slip) both on screw' and barrel's surface and transport is effected by shearing the fluid in a Couette flow pattern. Adhesion of fluid on screw and no interaction between fluid and the barrel (full-slip) will therefore cause no flow, but pure rotation.

Case 2: The fluid temporally adheres or slips. Transport is affected by alternate Coulomb's static or dynamic friction as a result of macroscopic density gradients under influence of gravitational forces. In circumstance of a reactor partially filled with granular bed, the fluid is raised in the tangential direction by the flights until reaching a specific torque. Afterwards, the fluid slips downwards into a lower position and is then raised again. This follows the standards of screw conveying mechanics where the volumetric flow is nearly proportional to filling degree as long as the rotation rate is kept constant.

Mixtures of these two cases are thinkable and flow characteristics depend on the properties of the fluid such as adhesion on solid bodies and viscous behaviour, the latter being mathematically expressed by several shear stress types like Newtonian, Ostwald-de Waele, and Bingham.

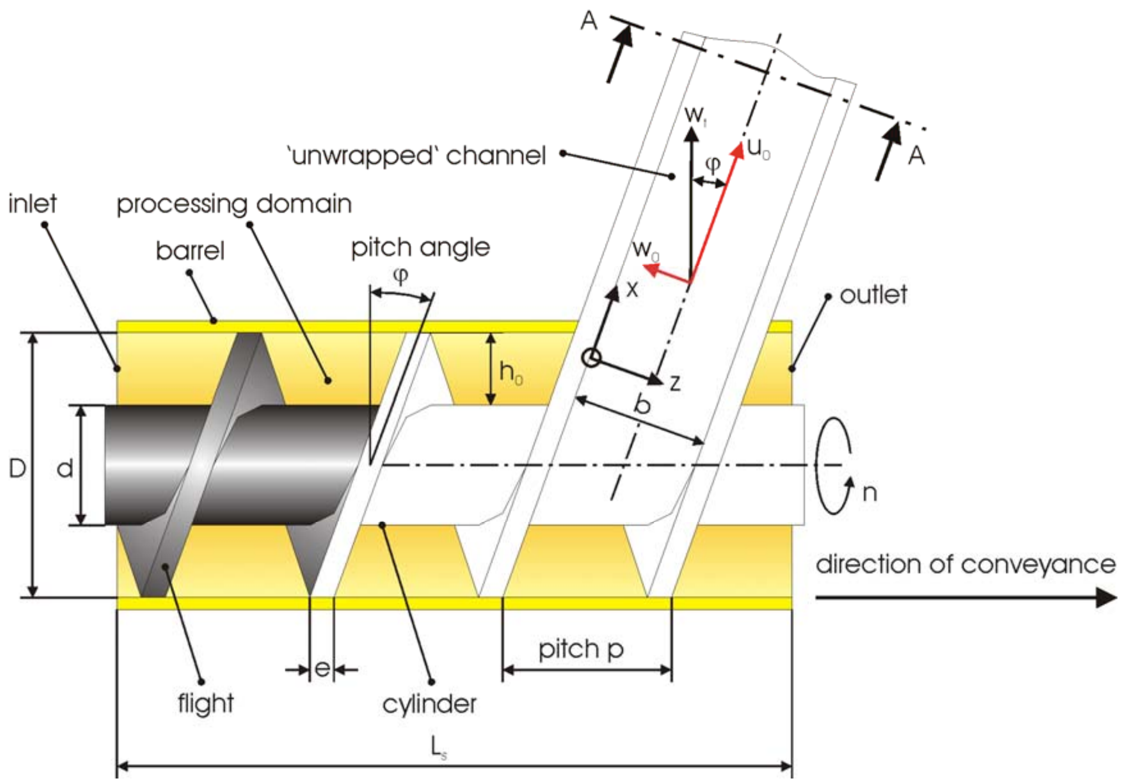

FIGURE 1: Transformation of the helical channel into a planar channel

Transformation of Geometry

For numerical reasons, the helical processing domain between screw and barrel has been transformed into a planar channel (**Fig. 1** and **Fig. 2**). Instead rotation of the screw, a translatoric movement of a plate right above the 'unwrapped' channel has been assumed. The relative tangential velocity between the tip of the flight and the plate is expressed by

$$w_t = \pi D n \qquad [1]$$

Which leads to the channel-fixed velocities in longitudinal direction u_0, which is responsible for axial transport, and the transverse velocity w_0 which generates recirculation of the fluid.

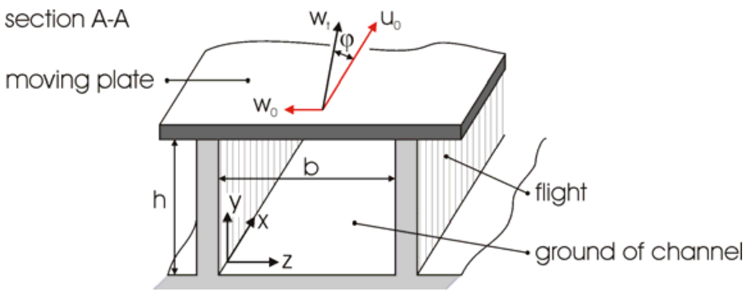

FIGURE 2: Planar channel dimensions and channel-fixed velocities.

Since u_0 is $\pi D / p$ times bigger than w_0, the transverse velocity has been neglected in the model. The outer pitch angle is calculated by

$$\varphi_{out} = \arctan\left(\frac{p}{\pi D}\right). \qquad [2]$$

For axial velocity of the moving plate we finally obtain

$$u_0 = w_t \cdot \cos(\varphi_{out}) = \pi D n \cdot \cos(\varphi_{out}). \qquad [3]$$

The length of the planar channel and the mean pitch angle are assumed to be

$$L_c = \frac{\pi(D+d)/2}{\cos(\varphi_m)} \cdot \frac{L_s}{p}, \qquad [4]$$

$$\varphi_m = \arctan\left(\frac{p}{\pi(D+d)/2}\right). \qquad [5]$$

The width of the channel is expressed by

$$b = \cos(\varphi_m)(p-e), \qquad [6]$$

taking into account thickness of the flight. For filling degrees $F < 1.0$ the processing domain is divided into two areas: The dense phase A in the bottom of the reactor, *e.g.* the packed bed and the gas phase B above (**Fig. 3**). Since behaviour of the gas phase is of lower interest and in order to save up computational time, only the volume fraction of the dense phase has been represented in the model. To incorporate variable filling degrees in the single phase model, the height of the channel has been adapted by

$$h = F \cdot h_o \,. \qquad [7]$$

Balance Equations

The balance equations for mass and momentum for the locally fixed finite volume are written

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\vec{w}\rho) \;\Rightarrow\; 0 = \nabla \cdot \vec{w} \qquad [8]$$

expecting density ρ to be constant and

$$\frac{\partial \rho \vec{w}}{\partial t} = -\nabla \cdot (\vec{w}\vec{w}\rho) - \nabla \cdot \quad - \nabla P + \rho \vec{g} \,. \qquad [9]$$

Given that the flow is isothermal, no energy equation needs to be solved.

Boundary conditions

As supplied before, transport characteristics strongly depend on momentum flux in the phase interface between the fluid and the solid parts of the reactor. Formulation of boundary conditions has been done in two steps: At first, transformation of boundary areas and second, setting of boundary type such as non-slip, slip or full slip.

Partitioning and Transformation of the Interface

Great care has been taken to accurately transform the geometric dimension of the phase interfaces. **Fig. 3** illustrates partitioning of the cylindrical shells**.**

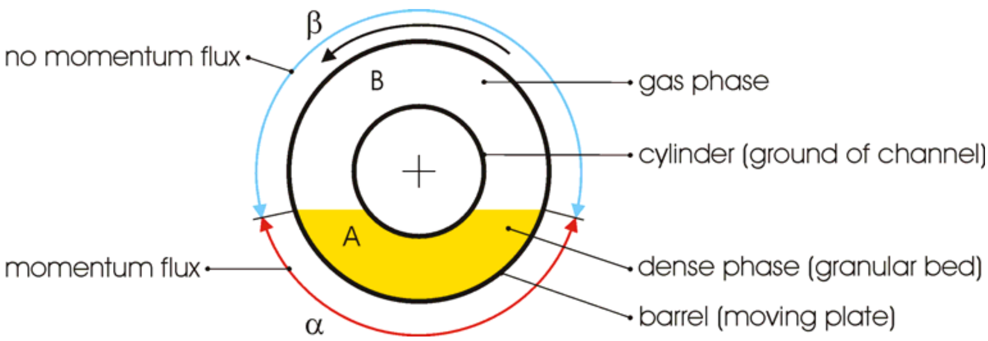

FIGURE 3: Partitioning of the phase interfaces

On barrel surface, momentum is transmitted over the range of angle α while no interaction takes place in the range of angle β. The ratio of α / β has been transferred onto the top of channel in longitudinal direction for each turn of the screw. In the same manner boundary conditions have been generated for the cylinder. Here, the length of the boundary face has been further multiplied by a factor d / D accounting for different surface dimensions of barrel and cylinder. Since section A is approximately proportional to degree of filling, the sidewalls of the channel, *i.e.* the flights, have not been partitioned (**Fig. 4**).

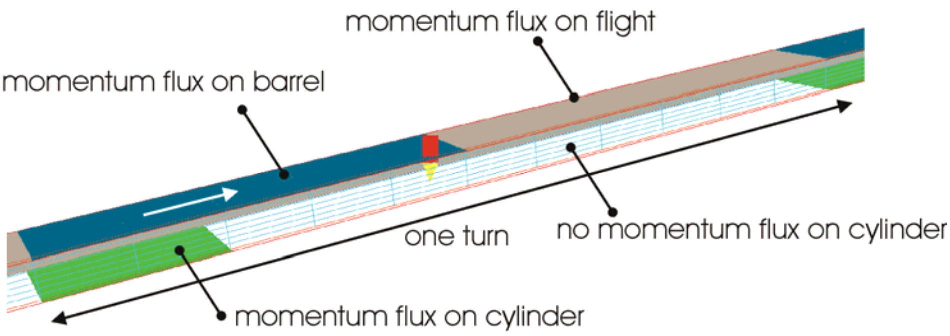

FIGURE 4: Assignment of interface partitioning for the planar channel, demonstrating a filling degree F = 0.4. The flight on the front side has been removed to allow for better insight.

Types of Boundary Conditions

In general the boundary conditions that have been comprised in the model can be classified into three categories:

1. No momentum flux at the interface, *i.e.* full-slip boundary. It has been used anytime there is no contact between the dense phase and the barrel or cylinder. **Fig.** 4 shows this type on top and ground of the channel's right side.
2. Momentum flux at the interface due to Coulomb's dynamic friction, *i.e.* slip boundary condition. This formulation has been adapted to the screw surface and may be adequate to handle slipping granular bed. Magnitude of momentum flux is calculated in dependence on normal forces at the screw surface and the friction coefficient.
3. Momentum flux at the interface by reason of fluid adhesion on the reactor surfaces, *i.e.* the non-slip boundary condition. This type has always been formulated for the moving wall, or more precisely, the top of the channel where the velocity of the fluid is directly set. Magnitude of momentum flux is therefore determined by the local shear stress which in turn is a function of shear strain and the viscosity coefficient of the fluid.

Boundary Conditions at Inlet and Outlet

At inlet and outlet of the channel, the pressures have been set equal and constant:

$$P_{in} = P_{out} = \text{constant} \qquad [10]$$

This has been implemented in the model by setting the pressure in the numerical cells touching the inlet- and outlet-plane. Since pressure in Phoenics™ is coupled with the balance equation for mass, cells at the inlet act as sources of mass while cells at the outlet act as sinks of mass. This behaviour is initiated by mass transport due to shear flow.

FLUID TYPES

Since viscous behaviour of the granular coals that will be finally used in the screw reactor process has not been exactly known, two kinds of fluids have been implemented to cover a wider range of possible flow: A Newtonian fluid and a Ostwald-de Waele fluid, the latter being a power-law fluid type. For an incompressible Newtonian fluid, the shear stress tensor can be written as

$$\boldsymbol{\tau} = -\eta\,\dot{\boldsymbol{\gamma}} = -\eta\,(\nabla\vec{w} + (\nabla\vec{w})^t) = -\eta \begin{bmatrix} 2\frac{\partial u}{\partial x} & \frac{\partial v}{\partial x}+\frac{\partial u}{\partial y} & \frac{\partial w}{\partial x}+\frac{\partial u}{\partial z} \\ \frac{\partial u}{\partial y}+\frac{\partial v}{\partial x} & 2\frac{\partial v}{\partial y} & \frac{\partial w}{\partial y}+\frac{\partial v}{\partial z} \\ \frac{\partial u}{\partial z}+\frac{\partial w}{\partial x} & \frac{\partial v}{\partial z}+\frac{\partial w}{\partial y} & 2\frac{\partial w}{\partial z} \end{bmatrix} \quad [11]$$

in which $\dot{}$ is the symmetrical rate of deformation tensor and $\nabla\vec{w}$ and $(\nabla\vec{w})^t$ are velocity gradient tensors. The dynamic viscosity η is a function of local temperature and pressure and is independent on the tensors τ and $\dot{\boldsymbol{\gamma}}$. In contrast to Newtonian fluid, the viscosity coefficient of the power-law fluid is assumed to be a function of the rate of deformation tensor and has been expressed by

$$\tau = -\eta(\dot{\boldsymbol{\gamma}})\,\dot{\boldsymbol{\gamma}} \quad [12]$$

in which $\eta(\dot{\boldsymbol{\gamma}})$ is assumed to be

$$\eta(\dot{\boldsymbol{\gamma}}) = \kappa\,\dot{\boldsymbol{\gamma}}^{1\text{-n}}. \quad [13]$$

κ is the fluid consistency index at a reference temperature and n is the flow behaviour index. By setting $n = 1$, we obtain the shear stress formulation of the Newtonian fluid and κ would match dynamic viscosity η. For $n < 1$ viscosity decreases with increasing rate of shear and the fluid is called pseudo plastic. For $n > 1$ viscosity increases with increasing rate of shear which is called dilatant. According to *Bird, Stewart and Lightfoot (2002)*, the scalar quantity $\dot{\gamma}$ is expected to be a function of the symmetrical rate of deformation tensor $\dot{\boldsymbol{\gamma}}$ in the form

$$\dot{\gamma} = \sqrt{\frac{1}{2}(\dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}})} = \sqrt{\frac{1}{2}\left(\sum_i\sum_j \dot{\gamma}_{ij}\ \dot{\gamma}_{ij}\right)} \text{ with } i, j = 1...3 \quad [14]$$

This leads to an expression

$$\dot{\gamma} = \sqrt{2\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial y}\right)^2 + 2\left(\frac{\partial w}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial x}+\frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial x}+\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial w}{\partial y}+\frac{\partial v}{\partial z}\right)^2}\ . \quad [15]$$

in which $\dot{\gamma}$ can be interpreted as a scalar shear strain of the finite volume. Sometimes, $\dot{\gamma}$ is quoted generation function in literature. As stated before, this function, which is implemented in Phoenics™ will be used to determine effective thermal conductivity of the packed bed later on. For flow of granular bed in the rotary kiln pyrolysis process, transport characteristics have been successfully described by *Schinkel* (2002) using a power-law formulation of shear stress with a flow behaviour index $n = 2$ and a consistency index κ as a function of particle diameter, bulk density and void fraction amongst other quantities. Therewith the non-cohesive granular bed of coals is expected to behave dilatant as well and in the one dimensional case shear stress may then be written

$$\tau_{yx} = -\kappa\left|\frac{\partial u}{\partial y}\right|^{n-1}\frac{\partial u}{\partial y} = -\kappa\left|\frac{\partial u}{\partial y}\right|\frac{\partial u}{\partial y}. \quad [16]$$

NUMERICAL COMPUTATION

The set of equation has been calculated transient up to steady state using commercial CFD-Code Phoenics™. A fully implicit upwind scheme has been used for discretisation of convective terms for reasons of numerical stability (*Rosten and Spalding*, 1987). The strictly orthogonal, structured grid is automatically generated within a self-written Fortran77 Code after the input of the geometric dimensions (D, d, Ls, p, e), filling degree F and rotation rate n. By comparison between numerical and analytic results for some selected cases of the fully filled reactor, approximately 150-200 in the yz-plane suffice for accurate reproduction of analytic velocity distributions. The calculation shows very good convergence behaviour.

MODELLING RESULTS

The velocity distributions in the yz-plane have been taken to deduce the mean volumetric flow in the longitudinal direction. Since flow properties of the coals still have to be determined, some fictional cases have been chosen to illustrate qualitative character of flow behaviour. The dimensionless results of numerical computation are summarised in **Fig**. 5. The diagonal graph reflects maximum possible flow which has been described by

$$\dot{V}_{\max} = \frac{\pi}{4}(D^2 - d^2) \cdot F \cdot p \cdot n, \qquad [17]$$

following the standards of screw conveyor mechanics.

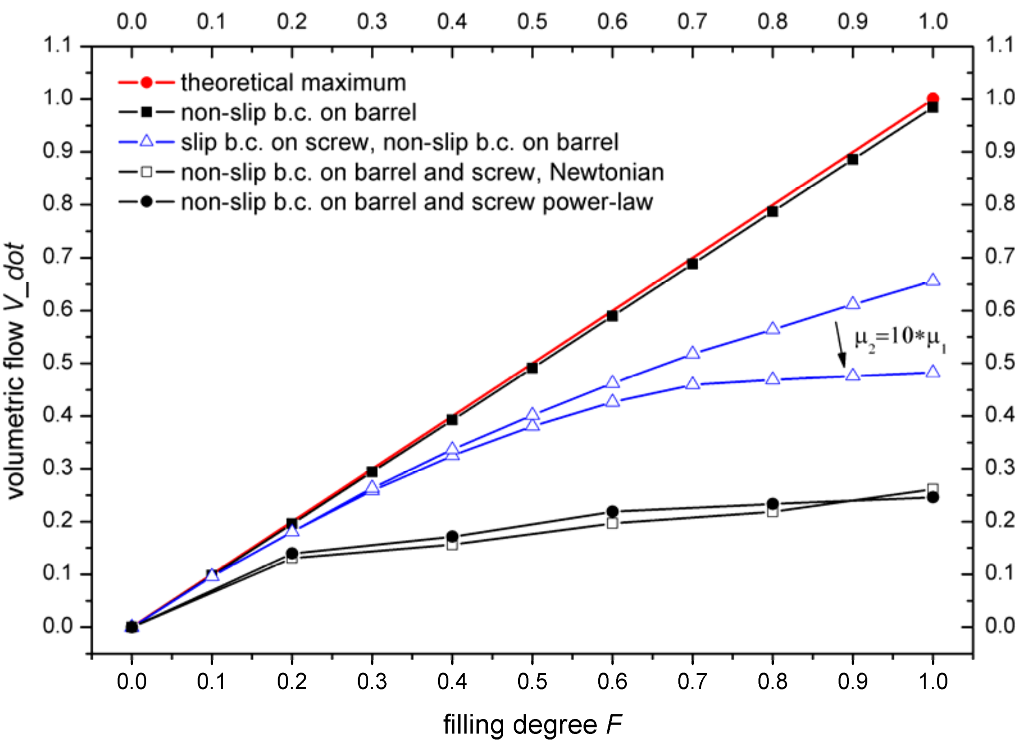

FIGURE 5: Volumetric flow for variable filling degree and different boundary conditions

This case is accurately represented by setting the momentum flux on the screw surfaces to zero. Thereby the fluid is not sheared and volumetric flow is expected to be

$$\dot{V} = u_0 \cdot b \cdot h \,. \qquad [18]$$

For full adhesion, i.e. non-slip boundary conditions, on barrel and screw, volumetric flow predicted by the model is dramatically lower, especially for higher filling degrees and irrespective of fluid type. This non-linear behaviour directly originates in the geometric dimensions of the boundary areas, both by adaptation of the channel height and the partitioning on barrel and cylinder. Although influence of fluid type seems to be negligible concerning mean volumetric flow $\dot{V}$, it still affects velocity distribution and therewith local effective thermal conductivity. It is interesting to mention that neither η nor κ has any impact on the velocity distributions, although it codetermines power consumption of the reactor.

The triangled graph demonstrates volumetric flow due to adhesion on barrel and Coulomb's dynamic friction on screw. The lower branch illustrates how flow is decreased when the friction coefficient is increased by factor 10. This combination of slip and non-slip boundary conditions is supposed to be the most adequate choice to model flow of the packed bed.

CONCLUSIONS

The basic transport mechanism in the partially filled single screw reactor has been studied by means of a single phase model. Slip and non-slip behaviour of incompressible, isothermal fluids have been represented by adequate formulation of boundary conditions. Volumetric flows predicted by the model for selected cases are reasonable. While differences in volumetric flow between Newtonian and power-law fluids seem negligible, the formation of velocity distribution will affect effective thermal conductivity. Due to the fully implicit upwind scheme and the usage of a structured, orthogonal grid, numeric calculation shows very good convergence behaviour. For future, flow properties of the packed coal bed will be determined and implemented in the model. Once the model is validated by experimental results, adaptations to model twin screw flow will be studied.

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