Created in COMSOL Multiphysics 6.0

2D Non-Newtonian Slot Die Coating

Introduction

Achieving uniform coating quality is important in several different industries: from optical coatings, semiconductor and electronics industry, through technologies utilizing thin membranes, to surface treatment of metals. Bad coating quality will compromise the performance of the products, or lead to complete failure in some cases.

Several different coating processes exist. This tutorial investigates the performance of a slot-die coating process, a so-called pre-metered coating method. In this process, the coating fluid is suspended from a thin slot die to a moving substrate. The final coating layer thickness is evaluated from the continuity relationship for a coating liquid. Therefore, the thickness of the liquid layer is determined by the slot gap, the coating fluid inlet velocity and the substrate speed.

The final goal of coating processes is to achieve a defect-free film of a desired thickness. However, manufacturing the uniform coating is not a trivial task, various flow instabilities or defects such as bubbles, ribbing, and rivulets are frequently observed in the process. The die geometry, the size of the slot and height above the substrate, together with the non-Newtonian fluid nature of the coating fluid are important to consider.

This tutorial demonstrates how to model the fluid flow in a polymer slot die coating process using the **Laminar Two-Phase Flow, Phase Field** interface and an inelastic non-Newtonian power law model for the polymer fluid.

Model Definition

MODEL GEOMETRY

A typical setup of the slot-die coating process is shown in Figure 1.

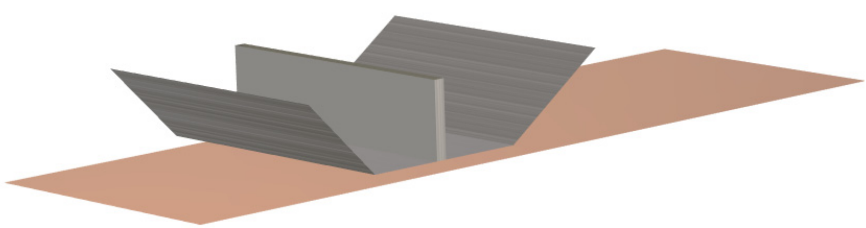

Figure 1: Typical geometry for a slot-die coating process with the slot die positioned over a substrate.

This model uses a 2D cross section of the die shown in Figure 1, assuming out-of-plane invariance. The inlet for the coating fluid is at the top of the die, as shown in Figure 2, and there are open boundaries at both ends. The bottom boundary is the coating substrate which is moving at the coating velocity.

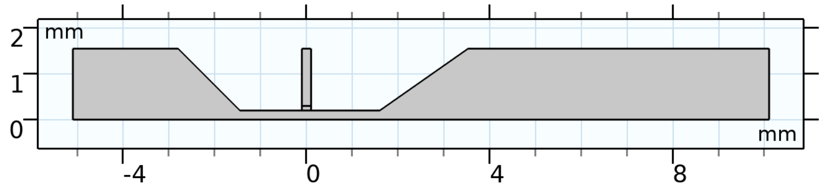

Figure 2: Model geometry. 2D cross section of a slot die.

The geometrical and material parameters in this model are taken from the Ref. 1.

DOMAIN EQUATIONS AND BOUNDARY CONDITIONS

The flow in this model is laminar, so a **Laminar Flow** interface will be used together with a **Phase Field** interface to track the interface between the air and the polymer fluid. The coupling of these two interfaces is handled by the **Two-Phase Flow, Phase Field** multiphysics interface. In this interface, you can select which constitutive relationship to use for each of the fluid phases. The air is specified as a Newtonian fluid, and the coating fluid is a non-Newtonian power law fluid.

The inlet fluid velocity is increases smoothly from 0 m/s to 0.1 m/s. Both the upstream and downstream boundaries of the model are specified as open boundaries. The corresponding inlet and outlet boundary conditions must also be set in the **Phase Field** interface together with the initial values for both fluids to correctly define the position of the initial interface. For the moving substrate, a moving wall boundary condition with a Navier-Slip condition is used.

Results and Discussion

The Figure 3 shows the evolution of the coating fluid interface for t = 0.03 s, t = 0.1 s, and t = 0.2 s.

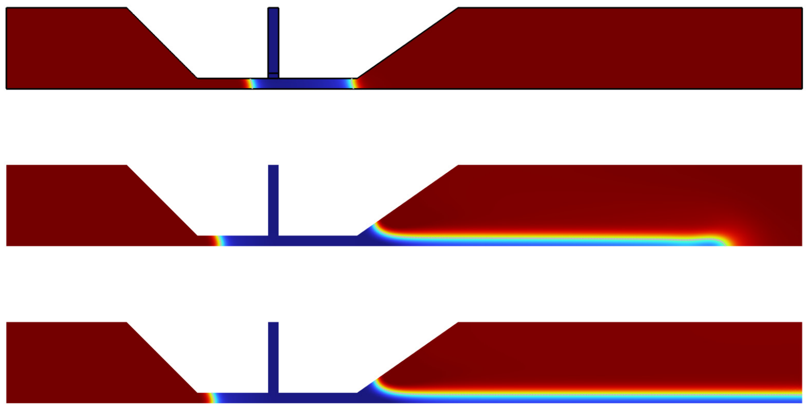

Figure 3: Coating fluid interface at t = 0.03 s, t = 0.1 s and t = 0.2 s (top to bottom).

The coating film attains a constant thickness downstream of the die at t = 0.2 s. The film forms upstream and downstream meniscii with the upstream and downstream walls of the die. As the substrate speed increases or the inlet velocity decreases, the upstream meniscus is pulled closer to the slot, eventually causing defects in the coating film. The evolution of the film thickness and position of the upstream meniscus as a function of time is shown in Figure 4.

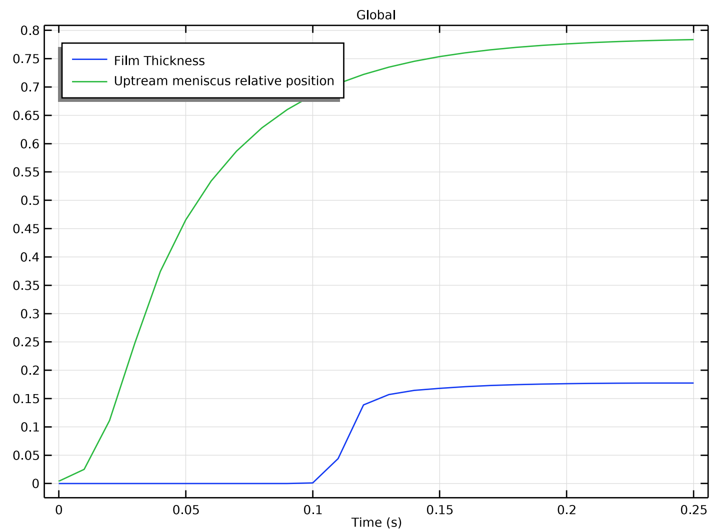

Figure 4: Film thickness and upstream meniscus position as a function of time.

By changing the geometry, the inlet velocity and wall velocity, it is easy to explore the sensitivity of the design parameters towards the film thickness and coating velocity for a variety of fluid properties in a fast and efficient manner.

Notes About the COMSOL Implementation

The default method for averaging the fluid properties across the interface between the two phases is linear with respect to the volume fraction. When working with fluids that have a large difference in viscosities, switching to a different averaging method increases the performance. In this example, the Heaviside averaging method is applied. The averaged viscosity is defined as

$$\mu = \mu_1 + (\mu_2 - \mu_1)\mathrm{H}\left(\frac{V_{f,2} - 0.5}{l_\mu}\right)$$

where V_2 is the volume fraction of fluid 2, μ_1 and μ_2 are the viscosities for fluid 1 and 2, respectively, and H is a smoothed Heaviside function. The default value of a mixing parameter l_μ is 0.8. In this model, the value of the l_μ is increase to 0.9. A lower value will sharpen the interface, but also increase the computation time.

Similarly, the averaged density is defined as

$$\rho = \rho_1 + (\rho_2 - \rho_1)\mathrm{H}\left(\frac{V_{f,2} - 0.5}{l_\rho}\right)$$

where ρ_1 and ρ_2 are the densities of fluid 1 and Fluid 2, respectively and l_ρ is a mixing parameter defining the size of the transition zone.

The default surface tension for the phase field model is evenly distributed across the fluid-fluid interface. In cases with a large difference in density between the two phases, significant spurious oscillations in the velocity field can occur for the lighter phase which results in smaller timesteps and longer computing time. Thus, it may be advantageous to shift the surface tension towards the heavy phase to avoid such oscillations. This is done by multiplying the surface tension force by

$$f_s = \frac{2}{(\rho_1 + \rho_2)}\left(\rho_1\mathrm{H}\left(\frac{V_{f,1} - 0.5}{d_{s,Fst}}\right) + \rho_2\mathrm{H}\left(\frac{V_{f,2} - 0.5}{d_{s,Fst}}\right)\right)$$

where $d_{s,Fst}$ is a mixing parameter defining the size of the transition zone.

In addition, this example demonstrates how to use an add-in to fit measured rheology data to a selected inelastic non-Newtonian fluid model. The add-in utilizes functionality from the Optimization Module. In case you do not have access to this module, you can skip the corresponding part of the instructions.

Reference

1. K.L. Bhamidipati, *Detection and elimination of defects during manufacture of high-temperature polymer electrolyte membranes,* PhD Thesis, Georgia Institute of Technology, 2011.

Application Library path: `Polymer_Flow_Module/Tutorials/slot_die_coating_2d`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select Physics** tree, select **Fluid Flow>Multiphase Flow>Two-Phase Flow, Phase Field>Laminar Flow**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics>Time Dependent with Phase Initialization**.

6 Click **Done**.

Load the model parameters from a text file.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `slot_die_coating_2d_parameters.txt`.

Create a step function to use for ramping up the inlet velocity. To improve convergence, define a smoothing transition zone to gently increase the inlet velocity from zero.

Step 1 (step1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Step**.

2 In the **Settings** window for **Step**, type `step1` in the **Function name** text field.

3 Locate the **Parameters** section. In the **Location** text field, type `0.01`.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type `0.02`.

Create the geometry by using a rectangle and a polygon.

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `W`.

4 In the **Height** text field, type `Hc`.

5 Locate the **Position** section. In the **x** text field, type `-W/2`.

6 In the **y** text field, type `H`.

Add an additional layer at the bottom of the channel. You will use it later to define the initial domain for the coating fluid.

7 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (mm)
Layer 1	0.1[mm]

8 Click **Build Selected**.

Polygon 1 (pol1)

1 In the **Geometry** toolbar, click **Polygon**.

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 In the table, enter the following settings:

x (mm)	y (mm)
-W/2	H
-W/2-W_ud	H
-W/2-W_ud-tan(alpha_u)*Hc	Hc+H
-W/2-L_u	Hc+H
-W/2-L_u	0
W/2+L_d	0
W/2+L_d	Hc+H
W/2+W_dd+tan(alpha_d)*Hc	Hc+H
W/2+W_dd	H

4 Click **Build Selected**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the resulting geometry to Figure 2.

DEFINITIONS

Next define integration operators. First define an integration coupling that integrates along the outlet boundary, to calculate the film thickness. Then define a coupling operator that integrates along the upstream die lip. You will use it later for the integration of the volume fraction along the boundary to evaluate the location of the upstream meniscus.

Integration 1 (intop1)

1. In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.
2. Right-click **Definitions** and choose **Nonlocal Couplings>Integration**.
3. In the **Settings** window for **Integration**, locate the **Source Selection** section.
4. From the **Geometric entity level** list, choose **Boundary**.
5. Select Boundary 16 only.

Integration 2 (intop2)

1. In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.
2. In the **Settings** window for **Integration**, locate the **Source Selection** section.
3. From the **Geometric entity level** list, choose **Boundary**.
4. Select Boundary 5 only.

ADD MATERIAL

Define the materials for the model — air and a coating fluid.

1. In the **Home** toolbar, click **Add Material** to open the **Add Material** window.
2. Go to the **Add Material** window.
3. In the tree, select **Built-in>Air**.
4. Click **Add to Component** in the window toolbar.
5. In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Coating Fluid

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
2. In the **Settings** window for **Material**, type `Coating Fluid` in the **Label** text field.

The physics interface and the chosen fluid model will suggest which material properties should be defined.

MULTIPHYSICS

Two-Phase Flow, Phase Field 1 (tpf1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Two-Phase Flow, Phase Field 1 (tpf1)**.

2 In the **Settings** window for **Two-Phase Flow, Phase Field**, locate the **Fluid 1 Properties** section.

3 From the **Fluid 1** list, choose **Air (mat1)**.

4 Locate the **Fluid 2 Properties** section. From the **Fluid 2** list, choose **Coating Fluid (mat2)**.

5 Find the **Constitutive relation** subsection. From the list, choose **Inelastic non-Newtonian**.

6 Locate the **Surface Tension** section. From the **Surface tension coefficient** list, choose **User defined**. In the σ text field, type `0.049`.

If you have the Optimization module in your license, you may use an add-in to calculate the parameters for the power law fluid model based on measurement data in this example. The instructions in the following section show you how to do this. If you do not have access to that license, you may just use the parameters m=7.77 and n=0.86 for the power law coefficients.

In the **Home** toolbar, click **Windows** and choose **Add-in Libraries**.

ADD-IN LIBRARIES

1 In the **Add-in Libraries** window, click **Refresh**.

2 In the tree, select **Polymer Flow Module> inelastic_non_newtonian_fluid_parameter_estimation**.

3 In the tree, select the check box for the node **Polymer Flow Module> inelastic_non_newtonian_fluid_parameter_estimation**.

4 Click **Done**.

ROOT

In the **Developer** toolbar, click **Add-ins** and choose **Inelastic Non-Newtonian Fluid Parameter Estimation>Inelastic Non-Newtonian Fluid Parameter Estimation**.

GLOBAL DEFINITIONS

Inelastic Non-Newtonian Fluid Parameter Estimation 1

1. In the **Model Builder** window, under **Global Definitions** click **Inelastic Non-Newtonian Fluid Parameter Estimation 1**.
2. In the **Settings** window for **Inelastic Non-Newtonian Fluid Parameter Estimation**, click **Load from File**.
3. Browse to the model's Application Libraries folder and double-click the file `slot_die_coating_2d_viscosity_input.txt`.

   Click **Create** to start the parameter estimation.

   The power law parameters can now be found in the global parameters table, and thus be used in the material node for the Coating Fluid.

MATERIALS

Coating Fluid (mat2)

1. In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Coating Fluid (mat2)**.
2. In the **Settings** window for **Material**, locate the **Material Contents** section.
3. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	1400	kg/m³	Basic
Fluid consistency coefficient	m_pow	m_powerLaw	Pa·s	Power law
Flow behavior index	n_pow	n_powerLaw	1	Power law

   To avoid having the optimization component in the model, use the **Clear** button in the add-in to clean up the model tree.

Now, set up the physics of the problem by defining the domain physics conditions and the boundary conditions.

LAMINAR FLOW (SPF)

Wall 2

1. In the **Model Builder** window, under **Component 1 (comp1)** right-click **Laminar Flow (spf)** and choose **Wall**.
2. Select Boundary 2 only.

3 In the **Settings** window for **Wall**, locate the **Boundary Condition** section.

4 From the **Wall condition** list, choose **Navier slip**.

5 Click to expand the **Wall Movement** section. Select the **Sliding wall** check box.

6 In the U_{w} text field, type `-U_wall`.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 Select Boundary 10 only.

3 In the **Settings** window for **Inlet**, locate the **Velocity** section.

4 In the U_0 text field, type `step1(t[1/s])*U_in`.

Open Boundary 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Open Boundary**.

2 Select Boundaries 1 and 16 only.

The initial interface between the coating fluid and air is automatically assigned to the boundaries between the two initial value domains. Set up the initial coating fluid domain in the inlet channel.

PHASE FIELD (PF)

Initial Values, Fluid 2

1 In the **Model Builder** window, under **Component 1 (comp1)>Phase Field (pf)** click **Initial Values, Fluid 2**.

2 Select Domain 3 only.

Wetted Wall 1

1 In the **Model Builder** window, click **Wetted Wall 1**.

2 In the **Settings** window for **Wetted Wall**, locate the **Wetted Wall** section.

3 In the θ_w text field, type `68.5[deg]`.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 In the **Settings** window for **Inlet**, locate the **Phase Field Condition** section.

3 From the list, choose **Fluid 2 (φ = 1)**.

4 Select Boundary 10 only.

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.

2 Select Boundaries 1 and 16 only.

Wetted Wall 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Wetted Wall**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Wetted Wall**, locate the **Wetted Wall** section.

4 In the θ_w text field, type `74[deg]`.

When working with fluids that have large viscosity and density ratios, switching from the default linear method for the properties averaging can increase the performance.

MULTIPHYSICS

Two-Phase Flow, Phase Field 1 (tpf1)

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog box, in the tree, select the check box for the node **Physics>Advanced Physics Options**.

3 Click **OK**.

4 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Two-Phase Flow, Phase Field 1 (tpf1)**.

5 In the **Settings** window for **Two-Phase Flow, Phase Field**, click to expand the **Advanced Settings** section.

6 From the **Density averaging** list, choose **Heaviside function**.

7 In the l_ρ text field, type `0.9`.

8 From the **Viscosity averaging** list, choose **Heaviside function**.

9 In the l_μ text field, type `0.9`.

The mixing parameter can be decreased to sharpen the interface, but that will increase the computation time for this example.

10 Select the **Shift surface tension force to the heaviest phase** check box.

To avoid spurious velocity and pressure oscillations due to the large density and viscosity ratios between the fluid, it can be advantageous to shift the surface tension force so that it is only applied in the heaviest phase. Note that this will reduce the computation time by a factor of two in this model.

If you want to inspect the progress of the fluids during the simulation, you can enable the plot while solving option in the **Step 2: Time Dependent** node. By calculating the initial values first, the solver sequence and default plots will be generated. In the following section you generate the default plot groups and use one of them for plotting the volume fraction while solving. Note that plot while solving in general will affect the computation time slightly since the plot needs to be updated in each timestep.

STUDY 1

In the **Study** toolbar, click **Get Initial Value**.

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, click to expand the **Results While Solving** section.

3 Select the **Plot** check box.

4 From the **Plot group** list, choose **Volume Fraction of Fluid 1 (pf)**.

5 From the **Update at** list, choose **Time steps taken by solver**.

6 Locate the **Study Settings** section. In the **Output times** text field, type `range(0,0.01,0.25)`.

7 In the **Study** toolbar, click **Compute**.

Examine the default plot at $t = 0.03$, 0.1, 0.2 (Figure 3)

RESULTS

Volume Fraction of Fluid 1 (pf)

1 In the **Model Builder** window, under **Results** click **Volume Fraction of Fluid 1 (pf)**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **0.03**.

4 In the **Volume Fraction of Fluid 1 (pf)** toolbar, click **Plot**.

5 From the **Time (s)** list, choose **0.1**.

6 In the **Volume Fraction of Fluid 1 (pf)** toolbar, click **Plot**.

7 From the **Time (s)** list, choose **0.2**.

8 In the **Volume Fraction of Fluid 1 (pf)** toolbar, click **Plot**.

Proceed to reproduce the plot of the film thickness and the upstream meniscus position Figure 4.

Film Thickness and Upstream Meniscus Position

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Film Thickness and Upstream Meniscus Position` in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 Right-click **Film Thickness and Upstream Meniscus Position** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

Expression	Unit	Description
`intop1(pf.Vf2)`	`mm`	`Film Thickness`
`intop2(pf.Vf2)/intop2(1)`	`1`	`Uptream meniscus relative position`

4 In the **Film Thickness and Upstream Meniscus Position** toolbar, click **Plot**.