

Slot-Die Coating with Channel Defect

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 premetered 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.

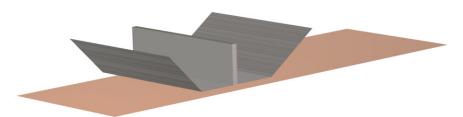


Figure 1: Typical geometry for a slot-die coating process with the slot die positioned over a substrate.

This example models the coating process in 3D where the inlet channel is obstructed (Figure 2).

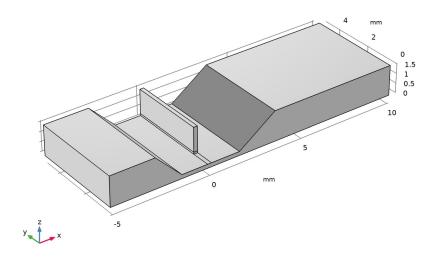
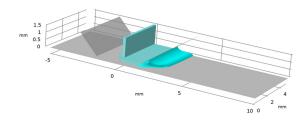


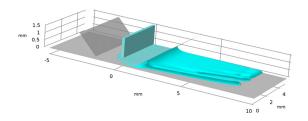
Figure 2: Model geometry.

More details about the model setup and COMSOL implementation can be found in the tutorial model 2D Non-Newtonian Slot-Die Coating.

Results

Figure 3 shows the evolution of the coating fluid interface for t = 0.05 s, t = 0.1 s, and t = 0.2 s.





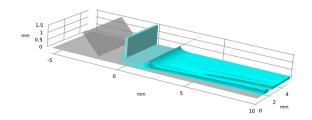


Figure 3: Fluid interface at t = 0.03 s, t = 0.1 s, and t = 0.2 s.

Figure 4 shows the variation of the film thickness across the outlet boundary. The channel defect leads to an uneven film thickness distribution. This can be partially mitigated by reducing the coating velocity.

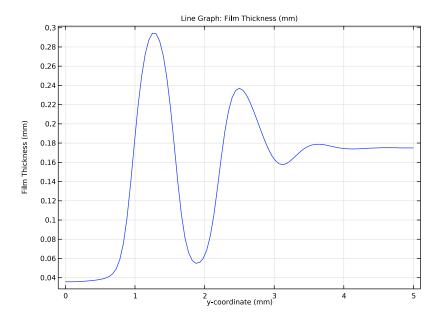


Figure 4: Coating film thickness across the outlet boundary.

Reference

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

Application Library path: Polymer_Flow_Module/Tutorials/
slot_die_coating_3d

Modeling Instructions

From the File menu, choose New.

NEW

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click 1 3D.
- 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 M Done.

GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
W	0.2[mm]	2E-4 m	Inlet width
Нс	1.35[mm]	0.00135 m	Inlet height
W_dd	1.5[mm]	0.0015 m	Die width downstream
W_ud	1.35[mm]	0.00135 m	Die width upstream
alpha_u	45[deg]	0.7854 rad	Upstream die angle
alpha_d	55[deg]	0.95993 rad	Downstream die angle
L_u	5[mm]	0.005 m	Upstream length
L_d	10[mm]	0.01 m	Downstream length
Н	0.2[mm]	2E-4 m	Channel height
Thickness	5[mm]	0.005 m	Thickness
U_wall	0.12[m/s]	0.12 m/s	Sliding wall velocity
U_in	0.1[m/s]	0.1 m/s	Inlet velocity
L_notch	1 [mm]	0.001 m	Length of channel end notch

GEOMETRY I

- I In the Model Builder window, expand the Component I (compl)>Geometry I node, then click Geometry 1.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose mm.

Work Plane I (wpl)

- I In the Geometry toolbar, click 🕌 Work Plane.
- 2 In the Model Builder window, click Work Plane I (wpl).
- 3 In the Settings window for Work Plane, locate the Plane Definition section.
- 4 From the Plane list, choose xz-plane.
- 5 Click Build All Objects.

Work Plane I (wp I)>Plane Geometry

In the Model Builder window, click Plane Geometry.

Work Plane I (wp I)>Rectangle I (r I)

- I In the Work Plane 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 **xw** text field, type -W/2.
- 6 In the yw text field, type H.
- 7 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (mm)
Layer 1	0.1

Work Plane I (wpl)>Polygon I (poll)

- I In the Work Plane toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Coordinates section.
- **3** In the table, enter the following settings:

xw (mm)	yw (mm)
-W/2	Н
-W/2-W_ud	Н
-W/2-W_ud-tan(alpha_u)*Hc	Hc+H

xw (mm)	yw (mm)
-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	Н

Extrude I (extI)

- I In the Model Builder window, right-click Geometry I and choose Extrude.
- 2 In the Settings window for Extrude, locate the Distances section.
- **3** In the table, enter the following settings:

Distances (mm) Thickness

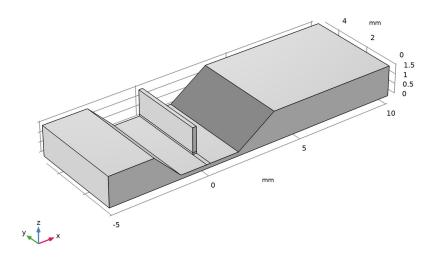
- 4 Select the Reverse direction check box.
- 5 Click **Build All Objects**.

Block I (blk I)

- I In the **Geometry** toolbar, click **Block**.
- 2 In the Settings window for Block, locate the Size and Shape section.
- 3 In the Width text field, type W.
- 4 In the **Depth** text field, type L_notch.
- 5 In the **Height** text field, type Hc.
- 6 Locate the Position section. In the z text field, type H.
- 7 In the \mathbf{x} text field, type -W/2.

Difference I (dif1)

- I In the Geometry toolbar, click Booleans and Partitions and choose Difference.
- **2** Select the object **ext1** only.
- 3 In the Settings window for Difference, locate the Difference section.
- 4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.
- **5** Select the object **blk1** only.



GLOBAL DEFINITIONS

Step I (step I)

- I In the Home toolbar, click f(X) Functions and choose Global>Step.
- 2 In the Settings window for Step, locate the Parameters section.
- 3 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.

Go to the Two-phase Flow, Phase Field Multiphysics-node to add a multiphase material and use the built in definitions to define the non-newtonian fluid properties for the coating fluid.

MULTIPHYSICS

Two-Phase Flow, Phase Field I (tpfI)

I In the Model Builder window, under Component I (compl)>Multiphysics click Two-Phase Flow, Phase Field I (tpfl).

- 2 In the Settings window for Two-Phase Flow, Phase Field, locate the Material Properties section.
- 3 Click Add Multiphase Material.

MATERIALS

Phase I (mpmat1.phase1)

- I In the Model Builder window, under Component I (compl)>Materials> Multiphase Material I (mpmatl) click Phase I (mpmatl.phasel).
- 2 In the Settings window for Phase, locate the Link Settings section.

ADD MATERIAL TO PHASE I (MPMATI.PHASEI)

- I Go to the Add Material to Phase I (mpmat1.phaseI) window.
- 2 In the tree, select Built-in>Air.
- 3 Click OK.

MATERIALS

Phase 2 (mpmat1.phase2)

- I In the Model Builder window, under Component I (compl)>Materials> Multiphase Material I (mpmat1) click Phase 2 (mpmat1.phase2).
- 2 In the Settings window for Phase, locate the Link Settings section.
- 3 Click Blank Material.

GLOBAL DEFINITIONS

Coating Fluid

- I In the Model Builder window, under Global Definitions>Materials click Material 2 (mat2).
- 2 In the Settings window for Material, type Coating Fluid in the Label text field.
- 3 Click to expand the Material Properties section. In the Material properties tree, select Fluid Flow>Inelastic Non-Newtonian>Power Law.
- 4 Click + Add to Material.
- 5 In the Material properties tree, select Basic Properties>Density.
- 6 Click + Add to Material.

7 Locate the Material Contents section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	1400	kg/m³	Basic
Fluid consistency coefficient	m_pow	7.77	Pa·s	Power law
Flow behavior index	n_pow	0.85	I	Power law

MATERIALS

Multiphase Material I (mpmat I)

- I In the Model Builder window, under Component I (compl)>Materials click Multiphase Material I (mpmatl).
- 2 In the Settings window for Multiphase Material, locate the Material Content section.
- **3** Click to select row number 1 in the table.
- 4 Click **Edit Mixing Rule**.
- 5 In the Edit Mixing Rule dialog box, choose Heaviside function from the Mixing rule list.
- **6** In the l_{mix} text field, type 0.9.
- **7** In the l_{mix} text field, type 0.9.
- 8 Click ... Next Row (Store Changes).
- 9 From the Mixing rule list, choose Heaviside function.
- 10 Click ... Next Row (Store Changes).
- II From the Mixing rule list, choose Heaviside function.
- I2 Click OK.

Since the materials have a large difference in density and viscosity, it is beneficial to sharpen the interface between these by using a heaviside mixing function for the respective properties.

- 13 Click the Show More Options button in the Model Builder toolbar.
- 14 In the Show More Options dialog box, select Physics>Advanced Physics Options in the tree.
- 15 In the tree, select the check box for the node Physics>Advanced Physics Options.
- 16 Click OK.

MULTIPHYSICS

Two-Phase Flow, Phase Field I (tpfl)

- I In the Model Builder window, under Component I (compl)>Multiphysics click Two-Phase Flow, Phase Field I (tpfI).
- 2 In the Settings window for Two-Phase Flow, Phase Field, click to expand the Advanced Settings section.
- 3 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 several hours in this model.

LAMINAR FLOW (SPF)

Inlet 1

- I In the Model Builder window, under Component I (compl) right-click Laminar Flow (spf) and choose Inlet.
- 2 Select Boundary 15 only.
- 3 In the Settings window for Inlet, locate the Velocity section.
- **4** In the U_0 text field, type $U_in*step1(t[1/s])$.

Open Boundary I

- I In the Physics toolbar, click **Boundaries** and choose **Open Boundary**.
- 2 Select Boundaries 1 and 23 only.

Symmetry I

- I In the Physics toolbar, click **Boundaries** and choose Symmetry.
- 2 Select Boundaries 5, 16, and 17 only.

Wall 2

- I In the Physics toolbar, click **Boundaries** and choose Wall.
- 2 Select Boundary 3 only.
- 3 In the Settings window for Wall, click to expand the Wall Movement section.
- 4 Select the Sliding wall check box.

5 Specify the $\mathbf{u}_{\mathbf{w}}$ vector as

U_wall*step1(t[1/s])	x
0	у
0	z

PHASE FIELD IN FLUIDS (PF)

Initial Values, Fluid 2

- I In the Model Builder window, under Component I (compl)>Phase Field in Fluids (pf) click Initial Values, Fluid 2.
- 2 Select Domain 3 only.

Inlet I

- I In the Physics toolbar, click **Boundaries** and choose Inlet.
- 2 Select Boundary 15 only.
- 3 In the Settings window for Inlet, locate the Phase Field Condition section.
- 4 From the list, choose Fluid 2 ($\varphi = 1$).

Wetted Wall 2

- I In the Physics toolbar, click **Boundaries** and choose Wetted Wall.
- 2 Select Boundary 3 only.
- 3 In the Settings window for Wetted Wall, locate the Wetted Wall section.
- **4** In the θ_w text field, type 74[deg].

Wetted Wall I

- I In the Model Builder window, click Wetted Wall I.
- 2 In the Settings window for Wetted Wall, locate the Wetted Wall section.
- **3** In the θ_w text field, type 68.5[deg].

Symmetry I

- I In the Physics toolbar, click **Boundaries** and choose Symmetry.
- 2 Select Boundaries 5, 16, and 17 only.

Outlet I

- I In the Physics toolbar, click **Boundaries** and choose **Outlet**.
- 2 Select Boundaries 1 and 23 only.

MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Sequence Type section.
- **3** From the list, choose **User-controlled mesh**.

Size

- I In the Model Builder window, under Component I (compl)>Mesh I click Size.
- 2 In the Settings window for Size, locate the Element Size section.
- **3** Click the **Custom** button.
- 4 Locate the Element Size Parameters section. In the Maximum element size text field, type 5.2E-2.

Size 1

In the Model Builder window, right-click Size I and choose Delete.

Compute the initial values. This will generate the default plots so that you can select which one to enable for plot while solving. Note that enabling plot while solving will increase the computation time for large models since time is spent on updating the selected plot in the graphical user interface after each solved time step. To reduce the computing time, disable plot while solving.

In the Study toolbar, click $\underset{=}{\overset{\cup}{\cup}}$ Get Initial Value.

STUDY I

Step 2: Time Dependent

- I In the Model Builder window, expand the Study I node, then 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 I (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 (0,0.05, .2).
- 7 In the Study toolbar, click **Compute**.

RESULTS

- I In the Model Builder window, click Results.
- 2 In the Settings window for Results, locate the Update of Results section.
- 3 Select the Only plot when requested check box.

Coating film

- I In the Home toolbar, click Add Plot Group and choose 3D Plot Group.
- 2 Right-click 3D Plot Group 4 and choose Rename.
- 3 In the Rename 3D Plot Group dialog box, type Coating film in the New label text field.
- 4 Click OK.

Volume 1

- I In the Model Builder window, right-click Coating film and choose Volume.
- 2 In the Settings window for Volume, locate the Expression section.
- 3 In the Expression text field, type 1.
- 4 Locate the Coloring and Style section. From the Coloring list, choose Uniform.
- 5 From the Color list, choose Cyan.
- 6 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.
- 7 In the Title text area, type Coating fluid.

Filter 1

- I Right-click Volume I and choose Filter.
- 2 In the Settings window for Filter, locate the Element Selection section.
- 3 In the Logical expression for inclusion text field, type pf. Vf2>0.5.
- 4 In the Coating film toolbar, click Plot.

Surface I

In the Model Builder window, right-click Coating film and choose Surface.

Selection 1

- I In the Model Builder window, right-click Surface I and choose Selection.
- 2 Select Boundary 2 only.
- 3 Click the Select All button in the Graphics toolbar.
- **4** Select Boundaries 6–13, 15, 16, and 18–21 only.

Surface I

I In the Model Builder window, click Surface I.

- 2 In the Settings window for Surface, locate the Coloring and Style section.
- **3** From the **Coloring** list, choose **Uniform**.
- 4 From the Color list, choose Gray.

Transparency I

- I Right-click Surface I and choose Transparency.
- 2 In the Settings window for Transparency, locate the Transparency section.
- **3** Set the **Transparency** value to **0.25**.

Surface I

- I In the Model Builder window, click Surface I.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type 1.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Surface 2

- I In the Model Builder window, right-click Coating film and choose Surface.
- 2 In the Settings window for Surface, locate the Expression section.
- **3** In the **Expression** text field, type 1.
- **4** Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the Coloring and Style section. From the Coloring list, choose Uniform.
- 6 From the Color list, choose Gray.

Selection 1

- I Right-click Surface 2 and choose Selection.
- **2** Select Boundary 3 only.
- 3 In the Coating film toolbar, click Plot.

Coating film

- I In the Model Builder window, under Results click Coating film.
- 2 In the Settings window for 3D Plot Group, locate the Plot Settings section.
- 3 Clear the Plot dataset edges check box.

To inspect the film thickness along the width of the outlet, you can use a nonlocal coupling operator, the linear projection operator. This operator integrates the projection of the expression on the surface toward the edge. Define this as shown in the following instructions.

DEFINITIONS

Linear Projection I (linproj I)

- I In the Definitions toolbar, click Nonlocal Couplings and choose Linear Projection.
- 2 In the Settings window for Linear Projection, locate the Source Selection section.
- 3 From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 23 only.
- 5 Locate the Source Vertices section. Click to select the Activate Selection toggle button.
- **6** Select Point 28 only.
- 7 Click to select the **Activate Selection** toggle button.
- **8** Select Point 30 only.
- **9** Click to select the **Activate Selection** toggle button.
- **10** Select Point 27 only.
- II Locate the **Destination Vertices** section. Click to select the **Destination Activate Selection** toggle button.
- **12** Select Point 27 only.
- **13** Click to select the **Activate Selection** toggle button.
- **14** Select Point 29 only.

Update the solution so that the newly defined operator is included.

STUDY I

In the Study toolbar, click C Update Solution.

RESULTS

Film thickness

- I In the Home toolbar, click Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, locate the Data section.
- **3** From the **Time selection** list, choose **Last**.
- 4 In the Label text field, type Film thickness.

Line Graph 1

- I Right-click Film thickness and choose Line Graph.
- **2** Select Edge 47 only.

- 3 In the Settings window for Line Graph, locate the y-Axis Data section.
- 4 In the Expression text field, type linproj1(pf.Vf2).
- 5 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 6 In the Expression text field, type y.
- 7 Locate the y-Axis Data section. From the Unit list, choose mm.
- 8 Locate the x-Axis Data section. From the Unit list, choose mm.
- 9 Locate the y-Axis Data section.
- 10 Select the **Description** check box. In the associated text field, type Film Thickness.
- II Click to expand the Quality section. From the Resolution list, choose No refinement.
- 12 In the Film thickness toolbar, click Plot.