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subject: Slot coating templates and tutorial for GOMA and SEAMS (GT-002.2)

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input records: SURFTANG, VELO_NORMAL, KINEMATIC, CAPILLARY, CA

Introduction

This tutorial assumes the user has gone through the beginner's training tutorial on GOMA and SEAMS. Specifically, it assumes the user has a strong familiarity with GOMA itself and the tools **`fastq`**, **`ex1ex2v2`**, **`aprepro`** and **`blot`**. If not, please go through that tutorial if you have it, or contact Duane Labreche (dalabre@sandia.gov) or Randy Schunk (prschun@sandia.gov) to get it.

We will introduce slot coating in two stages: first, a single layer slot coater and second, a two layer slot coater.

The key to running all of these problems is to obtain a good intial guess and then to know the details of the problem parameterization. This tutorial will try to cover all phases.

Single Layer Slot Coater

The key files in this directory, called "**`1lyr`**" under the "**`slot`**" subdirectory in the **`example_problems`** section of your master distribution, are **`slot_input`** and **`geometry`**. The **`geometry`** file describes the parameterization of the problem. The top of the file looks like:

```
$                inflow
$  -------------5        6---------------
$  \           |        |             /
$   \          |        |            /
$    \         |        |           /
$     \        |        |          /
$      \       |        3----------4       14
$       1 --------2
$
$
$  7-----------8--web-----9----------10-------8
$
$Geometrical paramterization:
$
$Define: x is parallel with the web, y is perpendicular to it.
$Gap [=] y1-y7, PERIOD! All rotation is done about point 1
$Lip 1: Specify y position of 2, relative to 1
$Lip 3: Specify y position of 3 and 4, relative to 1
$Slot [=] x6 - x5 == x3 - x2
$
$
$Also, x and y are just generic orthogonal directions here. Actually
$the model can be rotated with an angle alpha with the web, about point
$1, and so the distances specified above remain the same, because
$they will be relative to an imaginary line that goes through point 1
$and theta=0 means parallel to the web.
$
$
$Operating Conditions
$ Base set: vacuum = -400; surface tension=0.04; webspeed = 1.0
$$
$ Volumetric inflow rate/unit width m2/s {volumetric_inflow = .0002}
$ Vacuum backpressure    [=] Pa          {vacuum = -400.}
$ Substrate (web) speed  [=] m/s         {webspeed = 1.}
$ Viscosity (Newtonian)  [=] Pa-s        {viscosity = 0.1}
$ Density   (Newtonian)  [=] m^3/s       {density = 1000.}
$ Surface Tension        [=] N/m         {surface_tension = 0.04}
$
```

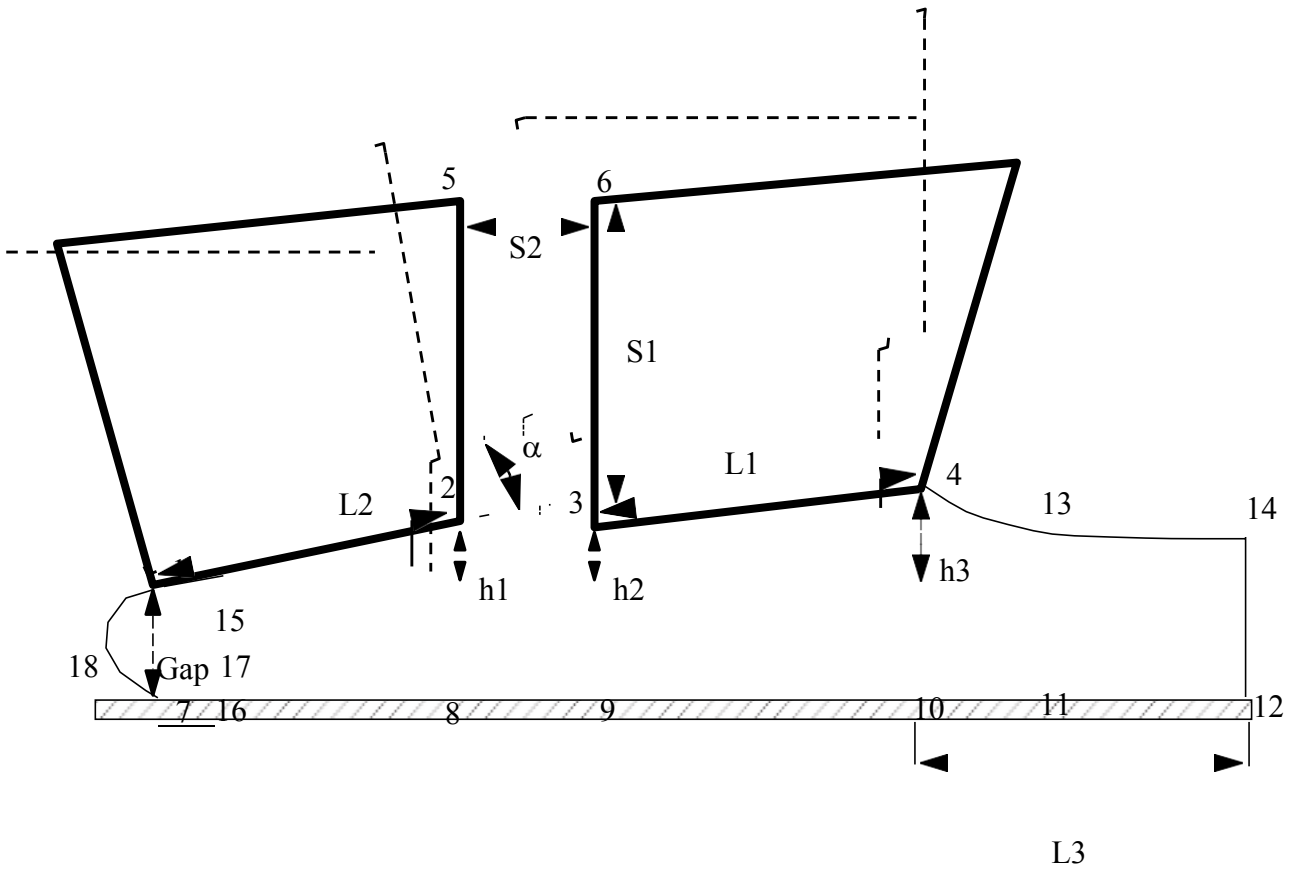
The first header comment attempts to explain some of the key points and other items, but the postscript file in the directory entitled **`slot.fm.ps`** has a more complete description. The operating conditions are fairly standard, as can be seen. All units are again in MKS. When making operating condition changes, use this file. After the operating condition section you will notice the Geometry description section. This section is the most important to understand.

```
$$
$Set Geometrical paramters (all parameters in MKS)
$$
$$ To make geometrical changes after having obtained a solution (btw
$$ see accompanying README file for details on how to obtain a solution)
$$ Please change the *_new parameter and leave the original geometry
$$ parameter the same because GOMA needs to know the difference and magnitude
$$ of the change. If you want to start with a different mesh, change both
```

```
$$ parameters and run fastq.
$$
$  Original mesh         You have changed
$  was built with:      it to:
$-----------------------------------------
$  {Gap = 0.0002 }      {Gap_new = 0.00020}
$  {h1  = 0.00006}      {h1_new  = 0.00006}
$  {h2  = 0.00004}      {h2_new  = 0.00004}
$  {h3  = 0.00001}      {h3_new  = 0.00001}
$  {alpha = 0.}         {alpha_new = 0.0}
$
$  {S2  = 0.0002}   {S2_new = 0.0002}
$  {S1  = 0.0005}   {S1_new = 0.0005}
$  {L2  = 0.0004}   {L2_new = 0.0004}
$  {L1  = 0.0004}   {L1_new = 0.0004}
$
$  {L3  = 0.0012}   {L3_new = 0.0012}
$
$ {heel_position = -0.000001}
$
$ {slip_length = 0.00003}
$
$$$
$Do a simple calculation
$$$
$ {inflow_speed = volumetric_inflow/S2_new}
$
$$Set mesh density
{no_elem_L2 = 12}
{no_elem_S1 = 6}
{no_elem_S2 = 6}
{no_elem_L1 = 10}
{no_elem_L3 = 15}
{no_elem_film = 7}
{no_elem_along_slip_length = 3}
```

The key geometrical quantities, like **`Gap, h1, h2, h3, alpha, S2, S1, L1, L3`**, are specified for the original mesh and also the updated or new conditions, during operation. As explained in the roll coating memo, GOMA is based on *displacements*. The **`*_new`** quantities are the geometrical changes that can be made in the file during a case study, i.e, after an initial solution has been obtained. It is important to understand here that GOMA solves for displacements of the nodes and not the actual coordinates as they evolve, and so coordinate DIFFERENCES must be tracked instead of absolute values. Hence, the boundary condition changes for Gap and die/substrate angle **`alpha`** alterations must have both the initial value and the desired value, the initial value being that at which the mesh was originally generated. Anyway, the geometrical parameterization looks like the figure to follow below.

You will notice that the die itself is parameterized such that it can be moved in and out towards the web and tilted about its heel for different angles of attack. If you scan down the geometry file you will see that all fastq geometry points have original and changed states defined. Then, with that as the case, then the coefficients a,b,c, and d



Parameters:

Gap: Distance between substrate and leading edge of upstream land

h1: Vertical distance (could be negative) between trailing edge of upstream land, and a Gap height above substrate, at zero angle α of attack.

h2: Vertical distance (could be negative) between leading edge of downstream land, and a Gap height above substrate, at zero angle α of attack.

h3: Vertical distance (could be negative) between trailing edge of downstream land, and a Gap height above substrate, at zero angle α of attack.

α: Angle of attack of die and substrate, with zero angle defining h1, h2, and h3

L1: Upstream land length

L2: Downstream land length

S1: slot length

S2: slot width

for the PLANE command conditions **`ax +by+cz+d = 0`** can be computed with Krammer's rule at the bottom of the file. In other words, when you make a geometrical change, the coefficients which parameterize the positions of the faces of the die are automatically computed. For fun, you should try changing some of the "original" geometrical

parameters and the "changed" parameters, keeping both the same, to different values and regenerating a mesh to get used to the parameterization. To generate the mesh you simply do the following:

```
fastq -a geometry
```

and then do an **m,p,g,p**, to see it, followed by a **,w** to write it out to a Genesis file. Don't forget to convert whatever that Genesis file is to an **exoII** file with **ex1ex2v2** and call it **slot.exoII**.

Slot coating initial guesses are considerably easier to obtain than roll coating initial guesses. The procedure here is quite simple. (1) Get a fixed grid solution using **VELO_NORMAL** conditions on the upstream and downstream menisci, (2) release the downstream meniscus by substituting **KINEMATIC, CAPILLARY**, and **SURFTANG** cards where appropriate, (3) postprocessing the results and picking off the pressure at the upstream meniscus, (4) setting the vacuum pressure to equal that pressure, and releasing the upstream meniscus. Both "release" stages do require some relaxation, as is diagrammed below. When picking the pressure off the fixed grid solution, or the single downstream mensicus solution is done simply by running "**blot**" on the **out.exoII** file, zooming in on the upstream meniscus, and contouring the pressure. Increase the number of contours with the **spectrum** command, or adjust to range with the **crange** command to get an accurate reading.

In fact, the contents of the README file accompanying the **1lyr** directory works pretty well. Try the recipe there.

The README file is:

```
First attain a fixed grid solution with

BC = VELO_NORMAL SS 23 0.
BC = VELO_NORMAL SS 6 0.

cards in lieu of

BC = KINEMATIC SS       23    0.
BC = CAPILLARY SS       23    {surface_tension} {vacuum} 0.
BC = CA              NS  700   1.000 0.0 -1.0 0.0
BC = CA              NS  100   0.600 0.0 1.0 0.0
BC = KINEMATIC SS        6    0.
BC = CAPILLARY SS        6    {surface_tension} 0.0 0.
BC = SURFTANG NS 1400 -1. 0. 0. {surface_tension}

cards.


Also set {surface_tension = 0.04} in "geometry" file.

i.e.,

BC = CAPILLARY   SS    6      {surface_tension} 0.0 0.
BC = SURFTANG    NS   1400     -1.0     0.0 0.0 {surface_tension}
```

cards.

```
goma -a -i slot_input -r 1.0
```

then save the solution

```
cp soln.dat contin.dat
```

Then release the downstream free surface by replacing
BC = VELO_NORMAL SS 6 0.

with

```
BC = KINEMATIC   SS     6      0.
BC = CAPILLARY   SS     6      {surface_tension} 0.0 0.
BC = SURFTANG_SCALAR NS 1400 {surface_tension}
```

and change "Initial Guess" card to "read"

Run goma:

```
goma -a -i slot_input
cp soln.dat contin.dat
```

Now release the upstream meniscus. Notice the {vacuum = -400}
to stabilize the meniscus. Here you need to relax a bit:

```
$$BC = VELO_NORMAL SS 23 0.
BC = KINEMATIC   SS     23      0.
BC = CAPILLARY   SS     23      {surface_tension} {vacuum} 0.
BC = CA          NS     700      1.000 0.0 -1.0  0.0
BC = CA          NS     100      0.600    0.0    1.0    0.0
```

```
goma -a -i slot_input -r 0.1 -n 10
cp soln.dat contin.dat
goma -a -i slot_input -r 0.2 -n 7
cp soln.dat contin.dat
goma -a -i slot_input
```

Notice the quadratic convergence on the last continuation step. Also
noteworthy is that we read off the pressure on the upstream meniscus
from the fixed grid case to be -1300 and added that as a backpressue
on sset 23

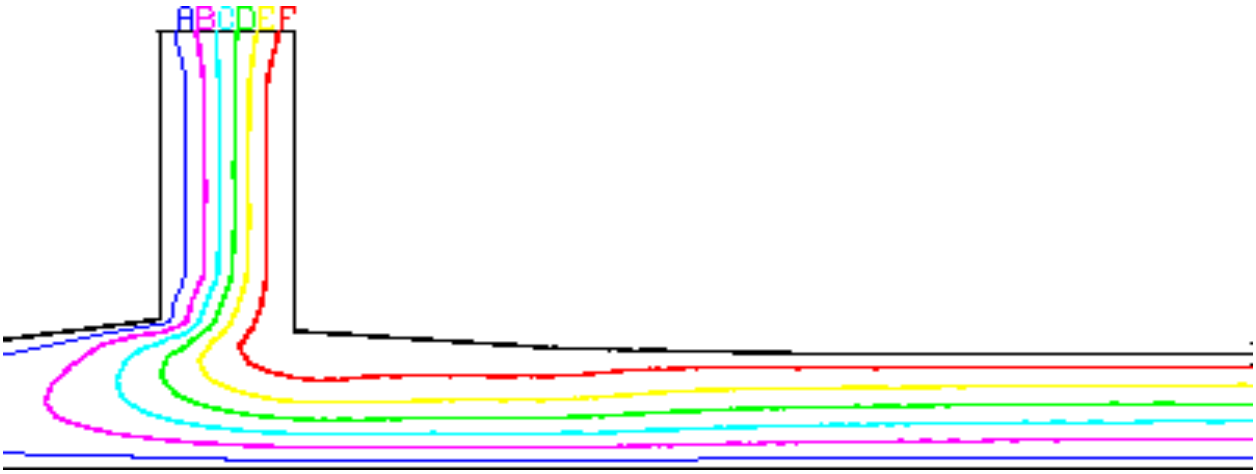
Also notice that you cannot take huge steps with the angle of attack
alpha.

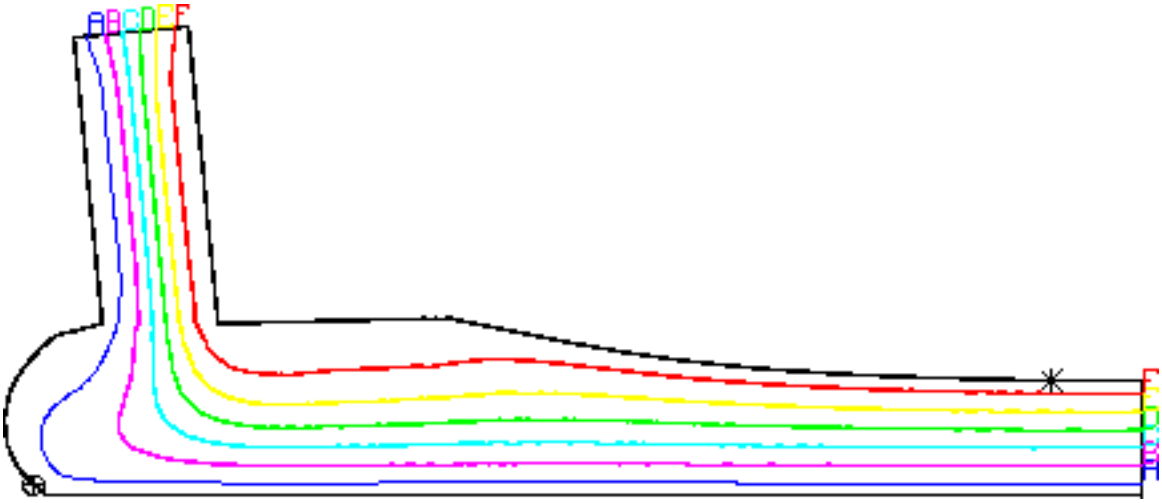
A little relaxation goes a long way. When making geometrical changes
keep them small or use relaxation, i.e., the good ol' -r switch.

Use and enjoy your new slot coater

prs (6/25/97)
dal (7/27/99)

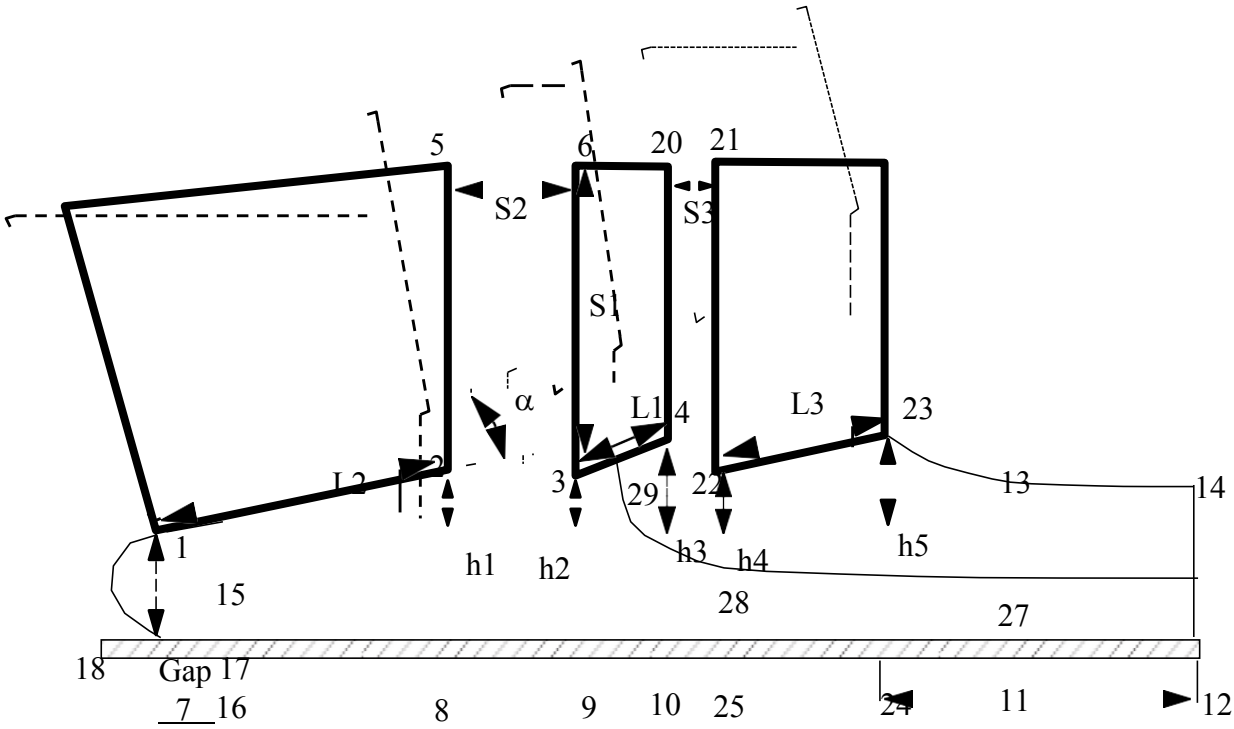
It is useful to do some exercises with the model to see how far you can push the parameters with the current setting and the current mesh. WARNING: Don't take too big of step in geometrical parameters unless using significant relaxation. For instance, changing the angle-of-attack from `alpha=0` to `alpha=0.1`, or `0.1` radians, and even with that you have to do 10 iterations at `-r = 0.1`, plus another 5 iterations at `-r=0.5`. Then I had to raise the backpressure to keep the upstream meniscus from being sucked in the nip. Anyway, things do work. Almost all parameters have been tested, but please provide feedback if you have it. The 0.1 angle of attack test leads to the following result:





Two-Layer Slot Template

The two-layer slot template is entitled `2lyr` under the "`slot`" subdirectory. The parameterization is very similar to the one layer case. It looks something like:



Parameters:

Gap: Distance between substrate and leading edge of upstream land L3

h1: Vertical distance (could be negative) between trailing edge of upstream land, and a Gap height above substrate, at zero angle α of attack.

h2: Vertical distance (could be negative) between leading edge of downstream land, and a Gap height above substrate, at zero angle α of attack.

h3: Vertical distance (could be negative) between trailing edge of downstream land, and a Gap height above substrate, at zero angle α of attack.

α: Angle of attack of die and substrate, with zero angle defining h1, h2, and h3

L1: Upstream land length

L2: Downstream land length

S1: slot length

The additional necessary information here is guidance on the interfacial boundary condition and the path of continuation to obtain an initial solution. This problem is substantially more difficult than the 1lyr case because of the interface contact line

between the layers. Its location on the center land is extremely sensitive to processing conditions. Just now the problem is set up for a flat-sided land whose angle can be changed etc. Note also that as in the one layer case the parameters for this problem have been consolidated at the top of the file "**geometry**" which is used to generate your mesh and all of the same concepts as discussed above apply here.

One particular warning is important here. YOU MUST START WITH HIGH SURFACE TENSION (~0.1) ON THE INTERFACE AND A 90 DEG. CONTACT ANGLE, THEN CONTINUE DOWN IN SURFACE TENSION. Of cource we are most interested in the case of zero surface tension.

As before get a fixed grid solution with the following boundary conditions AND the "Initial Guess" card set to "zero":

```
------
BC = VELO_NORMAL SS    23      0.
$$BC = KINEMATIC SS      23      0.
$$BC = CAPILLARY SS      23      {surface_tension1} {vacuum} 0.
$$BC = CA            NS  700       1.000 0. -1. 0.
$$BC = CA            NS  100       0.600 0. 1. 0.

$$ Down the downstream Meniscus

BC = VELO_NORMAL SS     6      0.
$$BC = KINEMATIC SS      6      0.
$$BC = CAPILLARY SS      6      {surface_tension2} 0. 0.
$$BC = SURFTANG NS      400    -1. 0. 0. {surface_tension2}
BC = VELO_TANGENT SS     8      0 0. 0. 0.

$$ Interface

BC = VELO_NORMAL SS     40      0.
$$BC = KINEMATIC SS      40      0.
$$BC = CAPILLARY SS      40      {.11} 0. 0.
$$BC = SURFTANG NS      260     -1. 0. 0. {.11}
$$BC = CA              NS    290     1.57 0. 1. 0.
```

Note that the additional complication here is the interface, or side set 40. For starters though we use the VELO_NORMAL condition as on the upstream and downstream menisci. Anyway, the following commands will get you this fixed grid solution

```
---------
goma -a -i slot_input
cp soln.dat contin.dat
```

Now set the "**Initial Guess**" card to "**read**" and change the interface boundary conditions (between layers on sset 40) as follows:

```
--------
$$BC = VELO_NORMAL SS     40      0
BC = KINEMATIC   SS     40      0.
BC = CAPILLARY   SS     40      {.11} 0. 0.
```

```
BC = SURFTANG   NS    260      -1. 0. 0.  {.11}
BC = CA                NS    290      1.57 0. 1. 0.
--------
```

Then run the following sequence:

```
goma -a -i slot_input -r 0.08 -n 40
cp soln.dat contin.dat
goma -a -i slot_input -r 0.1
cp soln.dat contin.dat
goma -a -i slot_input
```

Note that we have increased the surface tension to 0.11 N/m. After obtaining a solution you can drop that down to an insignificant value. Now you have a solution to the moving interface problem witha fixed external up- and downstream meniscus and a moving interface. Note that the initial conditions are such that the LAND between the two slots to be flat .

To release the downstream free surface:

```
--------
$$ Now the downstream Meniscus

$$BC = VELO_NORMAL SS 6 0.
BC = KINEMATIC   SS      6       0.
BC = CAPILLARY   SS      6       {surface_tension2} 0. 0.
BC = SURFTANG NS 400 -1. 0. 0. {surface_tension2}
BC = VELO_TANGENT SS     8      0 0. 0. 0.
------
```

Here you need run goma as follows:

```
goma -a -i slot_input -r 0.1
cp soln.dat contin.dat
goma -a -i slot_input
cp soln.dat contin.dat
```

Finally release the upstream meniscus the same way (SSET 23):

```
---------
$$BC = VELO_NORMAL SS 23 0.
BC = KINEMATIC   SS      23       0.
BC = CAPILLARY   SS      23       {surface_tension1} {vacuum} 0.
BC = CA          NS    700       1.000 0.0 -1.0  0.0
BC = CA          NS    100       0.600    0.0    1.0    0.0
--------
```

Here the vacuum is set to -800 up in the "geometry" file, as we had to use this the same way as we did in the single layer case.

Final note, when changing parameters here, you must take small steps and look at where the internal contact separation line wants to locate. Just now it is very limited as the land is flat. The next generation of this model will round that land and allow the separation line to travel up into either channel.