Updates to the pressure code to enable systems with parallel channels

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Main modifications

- Connectivity is specified in addition to dimensions in getGeometry function
- Graph tools are used to track connectivity and dimensions
- Solves for consistent mass flow across (in/out) each node

```
function myZero = massFlowRate(P, T, G)
mprickij = zeros(length(P), 1);
for i = 1:numedges(G)
    % Channel info
    ni = G.Edges.EndNodes(i, 1);
                                     % start node
    nj = G.Edges.EndNodes(i, 2);
                                     % end node
    LWH = [G.Edges.Length(i);
       G.Edges.Width(i);
       G.Edges.Height(i)];
                                      % segment dimensions
    % Compute mass flow rate across segment
    mdot_j1_j2 = compute_mprickij(LWH, P(ni), P(nj), T);
    % Add to node sums (inflow - outflow)
    mprickij(ni) = mprickij(ni) - mdot jl j2;
    mprickij(nj) = mprickij(nj) + mdot_j1_j2;
% Trim off inlet and outlet nodes as pressures there are known
inletnode = G.Edges.EndNodes(find(G.Edges.ConnectsIn == 1, 1), 1);
outletnode = G.Edges.EndNodes(find(G.Edges.ConnectsOut == 1, 1), 2);
mprickij([inletnode, outletnode]) = [];
% Mass flow rate should be constant across segment junctions
f = 1e10;
myZero = f * mprickij;
end
```

```
L56
function G = getGeometry(geom type)
id = geom type;
                                                                                            L23
switch id
   case 'wellmixed'
       disp('ID: Well-mixed')
                                                 L67
       % Channel lengths (m)
       L23 = 500e-6;
       L34 = 70e-6;
       L44 = 180e-6;
       L56 = L23;
       L67 = 21e-3:
       Lij = [L23; L34; L44; L34; L56; L67];
                                                      Mass flow rate: 1.2e-12 kg/s
       % Channel heights (m)
       h23 = 100e-9;
       h34 = 100e-9;
       h44 = 100e-9;
       h56 = 100e-9;
       h67 = 60e-6:
       Hii = [h23; h34; h44; h34; h56; h67];
       % Channel widths (m)
       w23 = 10e-6;
       w34 = 10e-6;
       w44 = 120e-6;
       w56 = 10e-6;
       w67 = 150e-6;
       Wij = [w23; w34; w44; w34; w56; w67];
       % Channel connectivity (channel connects start node to end node)
       C = zeros(length(Lij), 2);
       C(:, 1) = [1, 2, 3, 4, 5, 6]; % Start node
       C(:, 2) = [2, 3, 4, 5, 6, 7]; % End node
       % Store this info as a directed graph
       G = digraph(C(:, 1), C(:, 2), Lij * le3);
       G.Edges.Length(findedge(G,C(:, 1), C(:, 2))) = Lij;
       G.Edges.Width(findedge(G,C(:, 1), C(:, 2))) = Wij;
       G.Edges.Height(findedge(G,C(:, 1), C(:, 2))) = Hij;
```

L44

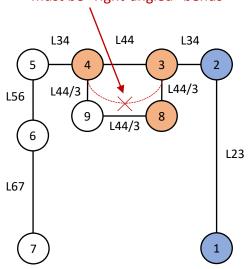
L34

L34

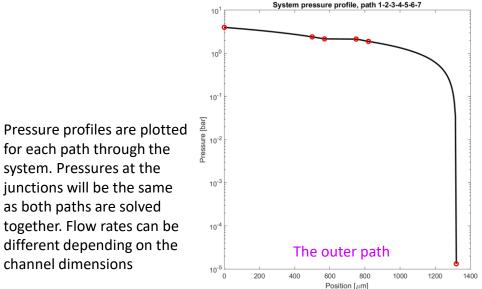
Eg1: One parallel channel

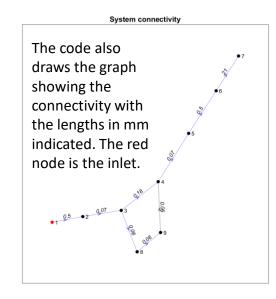
```
case 'parallel 1'
   disp('ID: Parallel 1')
   % Channel lengths (m)
   L23 = 500e-6;
   L34 = 70e-6;
   L44 = 180e-6;
   L56 = L23;
   L67 = 21e-3;
   Lij = [L23; L34; L44;
       L44/3; L44/3; L44/3; % Add one copy of the L44 segment
        L34; L56; L67];
   % Channel heights (m)
   h23 = 100e-9;
   h34 = 100e-9;
   h44 = 100e-9;
   h56 = 100e-9;
   h67 = 60e-6:
   Hij = [h23; h34; h44;
       h44; h44; h44;
       h34; h56; h67];
   % Channel widths (m)
   w23 = 10e-6;
   w34 = 10e-6;
                                     Node 3 is connected to node 4
   w44 = 120e-6;
   w56 = 10e-6:
   w67 = 150e-6;
                                     Node 3 is connected to node 8
   Wij = [w23; w34; w44;
       w44; w44; w44;
        w34; w56; w67];
   % Channel connectivity
                          (channel connects start node to end node)
   C(:, 1) = [1, 2, 3, 3, 8, 9, 4, 5, 6]; % Start node
   C(:, 2) = [2, 3, 4, 8, 9, 4, 5, 6, 7]; % End node
   % Store this info as a directed graph
   G = digraph(C(:, 1), C(:, 2), Lij * le3);
   G.Edges.Length(findedge(G,C(:, 1), C(:, 2))) = Lij;
   G.Edges.Width(findedge(G,C(:, 1), C(:, 2))) = Wij;
   G.Edges.Height(findedge(G,C(:, 1), C(:, 2))) = Hij;
```

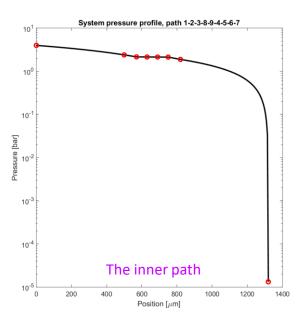
NB: no two channels can share the same two nodes so there must be "right-angled" bends



Mass flow rate: 1.2e-12 kg/s w 50/50 split in parallel part







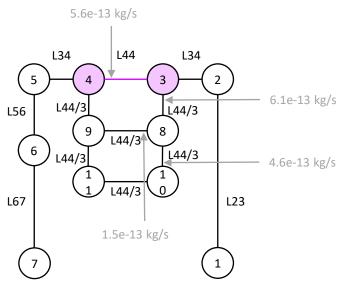
for each path through the system. Pressures at the junctions will be the same as both paths are solved together. Flow rates can be different depending on the

channel dimensions

Node 1 is connected to node 2

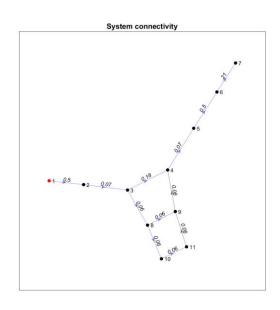
Eg2: Two parallel channels

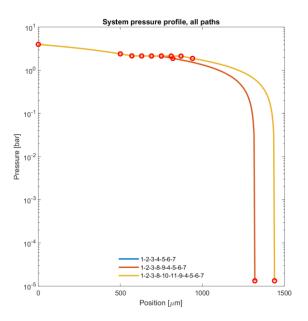
```
case 'parallel 2'
   disp('ID: Parallel 2')
   % Channel lengths (m)
   L23 = 500e-6;
   L34 = 70e-6:
   L44 = 180e-6;
   L56 = L23;
   L67 = 21e-3;
   Lij = [L23; L34; L44;
       L44/3; L44/3; L44/3; % Add two copies of the L44 segment in
       L44/3; L44/3; L44/3; % parallel, divided where they bend
       L34; L56; L67];
   % Channel heights (m)
   h23 = 100e-9;
   h34 = 100e-9;
   h44 = 100e-9;
   h56 = 100e-9;
   h67 = 60e-6;
   Hij = [h23; h34; h44;
       h44; h44; h44;
       h44; h44; h44;
                          Node numbering is arbitrary
       h34; h56; h67];
                         but the ordering of the channel
   % Channel widths (m)
                            dimensions in Lij, Hij, Wij
   w23 = 10e-6:
   w34 = 10e-6;
                           should match the rows in C
   w44 = 120e-6;
   w56 = 10e-6;
   w67 = 150e-6;
   Wij = [w23; w34; w44;
       w44; w44; w44;
       w44; w44; w44;
       w34; w56; w67];
   % Channel connectivity (channel connects start node to end node)
   C = zeros(length(Liv), 2);
   C(:, 1) = [1, 2, 3, 3, 8, 9, 8, 10, 11, 4, 5, 6]; % Start node
   C(:, 2) = [2, 3, 4, 8, 9, 4, 10, 11, 9, 5, 6, 7]; % End node
   % Store this info as a directed graph
   G = digraph(C(:, 1), C(:, 2), Lij * le3);
   G.Edges.Length(findedge(G,C(:, 1), C(:, 2))) = Lij;
   G.Edges.Width(findedge(G,C(:, 1), C(:, 2))) = Wij;
   G.Edges.Height(findedge(G,C(:, 1), C(:, 2))) = Hij;
```



Mass flow rate: 1.2e-12 kg/s w split as indicated

Plotting all profiles on the same axis shows that the outer path (connecting nodes 10 and 11) is longer





Eg3: Two parallel channels

```
case 'parallel 3'
   disp('ID: Parallel 3')
   % Channel lengths (m)
   L23 = 500e-6;
   L34 = 70e-6;
   L44 = 180e-6;
   L56 = L23:
   L67 = 21e-3;
   Lij = [L23; L34;
                                                  L34
                                                                          L34
       L44/3; L44/3; L44/3;
       L44/3; L44/3; L44/3;
       L34; L56; L67];
   % Channel heights (m)
                                         L56
   h23 = 100e-9;
   h34 = 100e-9;
   h44 = 100e-9;
   h56 = 100e-9:
   h67 = 60e-6:
                                                                                   L23
   Hij = [h23; h34;
       h44; h44; h44;
       h44: h44: h44:
                                         L67
       h34; h56; h67];
   % Channel widths (m)
   w23 = 10e-6;
   w34 = 10e-6;
   w44 = 120e-6;
   w56 = 10e-6:
                                             Mass flow rate: 1.2e-12 kg/s w
   w67 = 150e-6;
   Wij = [w23; w34;
                                                50/50 split in parallel part
       w44; w44; w44;
       w44; w44; w44;
       w34; w56; w67];
   % Channel connectivity (channel connects start node to end node)
   C = zeros(length(Lij), 2);
   C(:, 1) = [1, 2, 3, 8, 9, 3, 10, 11, 4, 5, 6]; % Start node
   C(:, 2) = [2, 3, 8, 9, 4, 10, 11, 4, 5, 6, 7]; % End node
   % Store this info as a directed graph
   G = digraph(C(:, 1), C(:, 2), Lij * le3);
   G.Edges.Length(findedge(G,C(:, 1), C(:, 2))) = Lij;
   G.Edges.Width(findedge(G,C(:, 1), C(:, 2))) = Wij;
   G.Edges.Height(findedge(G,C(:, 1), C(:, 2))) = Hij;
```

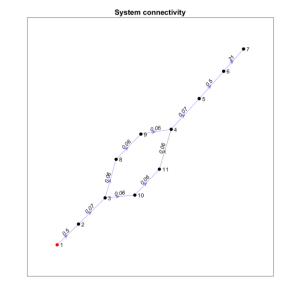
This table is printed out so you can check the dimensions are correct. Every row corresponds to one channel.

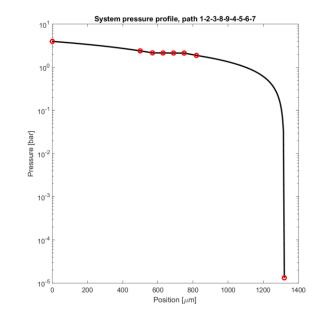
	rallel_3		s) and wei	.ghts (lengt	hs):		
EndNodes		Weight	Length	Width	Height	ConnectsIn	ConnectsOut
_							
1	. 2	0.5	0.0005	1e-05	le-07	1	0
2	3	0.07	7e-05	1e-05	le-07	0	0
3	8	0.06	6e-05	0.00012	1e-07	0	0
3	10	0.06	6e-05	0.00012	le-07	0	0
4	5	0.07	7e-05	1e-05	le-07	0	0
5	6	0.5	0.0005	1e-05	1e-07	0	0
6	7	21	0.021	0.00015	6e-05	0	1
8	9	0.06	6e-05	0.00012	le-07	0	0
9	4	0.06	6e-05	0.00012	le-07	0	0
10	11	0.06	6e-05	0.00012	le-07	0	0

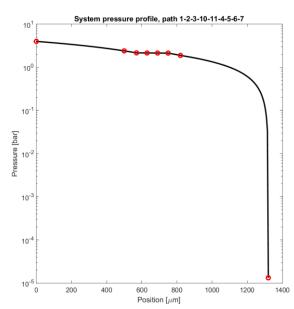
0.00012

1e-07

0.06







Comments

Pressures

- It is important that the initial guess for the pressure profile is reasonable. This is more difficult than in the linear case, because the pressure needs to drop between successive nodes. I added a function called *setPressures* to interpolate between the inlet and outlet pressures across each path and then average for nodes that occur in multiple paths.
- Since the ordering of the nodes is arbitrary, the inlet and outlet nodes do not need to have the smallest and largest node numbers (see examples on the previous slides where I chose to number the outer path first and the outlet node is node 7/11). I added the function reorder to put the specified initial and final pressures in the correct places in the pressure vector to match their node numbers.

Numerical stability

- I have tested the examples in the previous slides, and I believe the code should also work for a wider range of configurations (e.g., all the channels don't have to diverge and reconverge at the same pair of nodes). However, this assumption is untested so please let me know if it breaks under any configuration. I can imagine cases where it finds a negative mass flow or pressure solves the equations.
- I noticed in testing it that sometimes there is a tiny (order 1e-15) imaginary component in the pressures. I have clipped that off, but I added a warning in case it gets significant. Please let me know if you ever see that happening.