

# Example models for ruminant digestion and metabolism



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# Intro to Molly

## Representation of milk production

### Short demo using BST

## Exercise

#### WEBSITE:

<http://www.vmtrc.ucdavis.edu/laboratories/metabolic/molly.cfm>

#### Publications:

Baldwin RL, France J, Gill M. 1987. Metabolism of the lactating cow I-III.  
J Dairy Research 54:77-145.

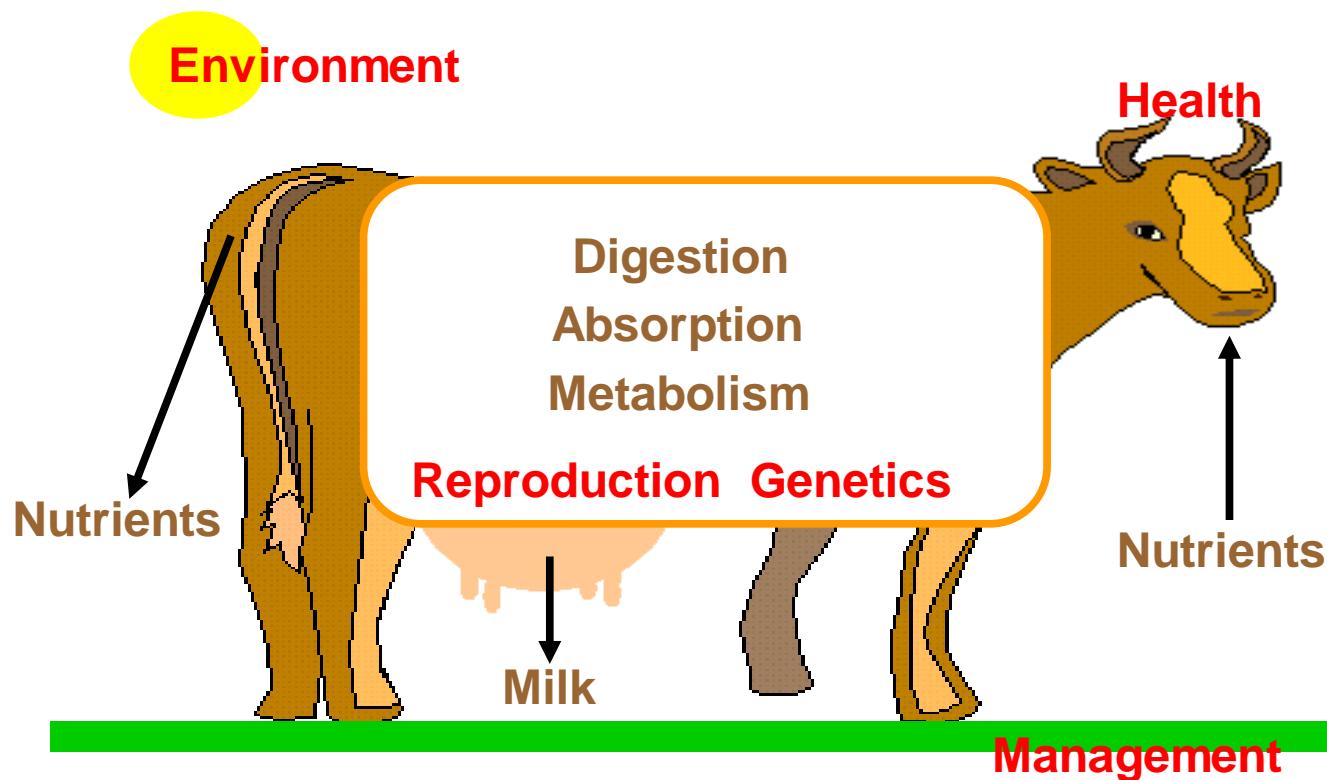
Baldwin RL. 1995. Modeling ruminant digestion and metabolism.  
Chapman & Hall:London.

Johnson HA, Maas JA, Calvert CC, Baldwin RL. 2008. Use of computer  
simulation to Teach systems approach to Nutrition and Metabolism.  
JAS 86:483-499

Neal & Thornley 1983 J Ag Sci Cambridge 101:389-400

# OBJECTIVE

Bridge gap between basic knowledge  
of cow digestion and metabolism,  
and animal performance



# **State Variables**

## **Animal Element**

Amino acids

(Lys His Met/Cys Other)

Glucose

Acetate

Fatty Acids

Adipose TG

Body Protein

Visceral Protein

Uenz

Milk lactose

Milk Protein

Milk Fat

Milk

## **Digestive Element**

Large Particles

Small Particles

Microbes

Rumen VFAs

DMI

Soluble Ash

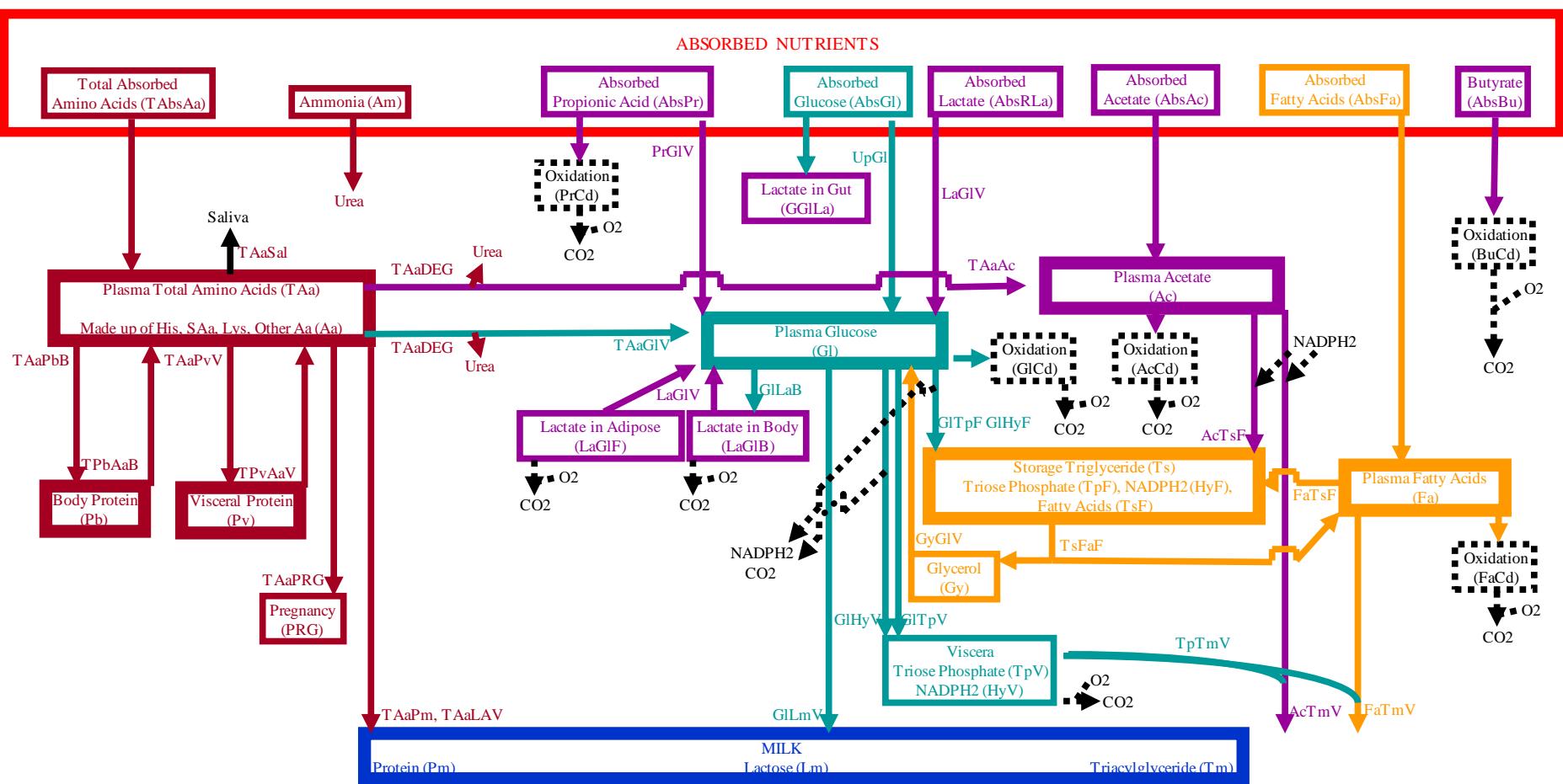
Cellulose

Hemicellulose

Soluble, Insoluble Protein

Soluble Carbohydrates

Alpha, Beta Hexoses



# Equations

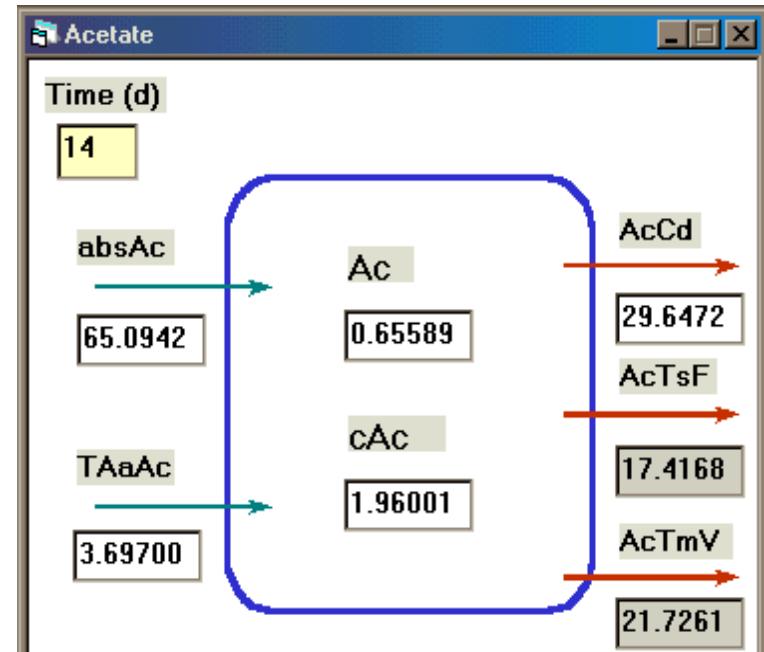
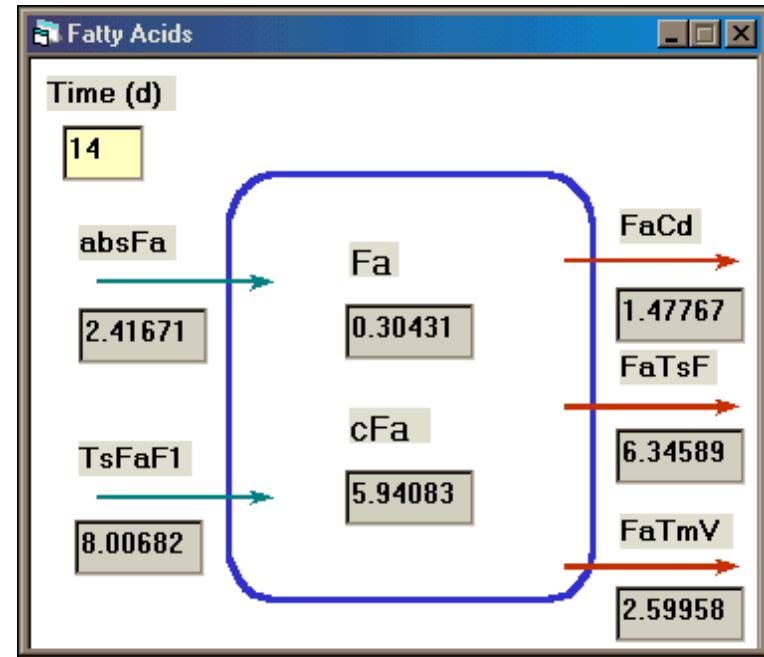
$$\frac{dFa}{dt} = absFa + TsFaF1 - FaTsf - FaTmV - FaCd$$

Units = Mol/d

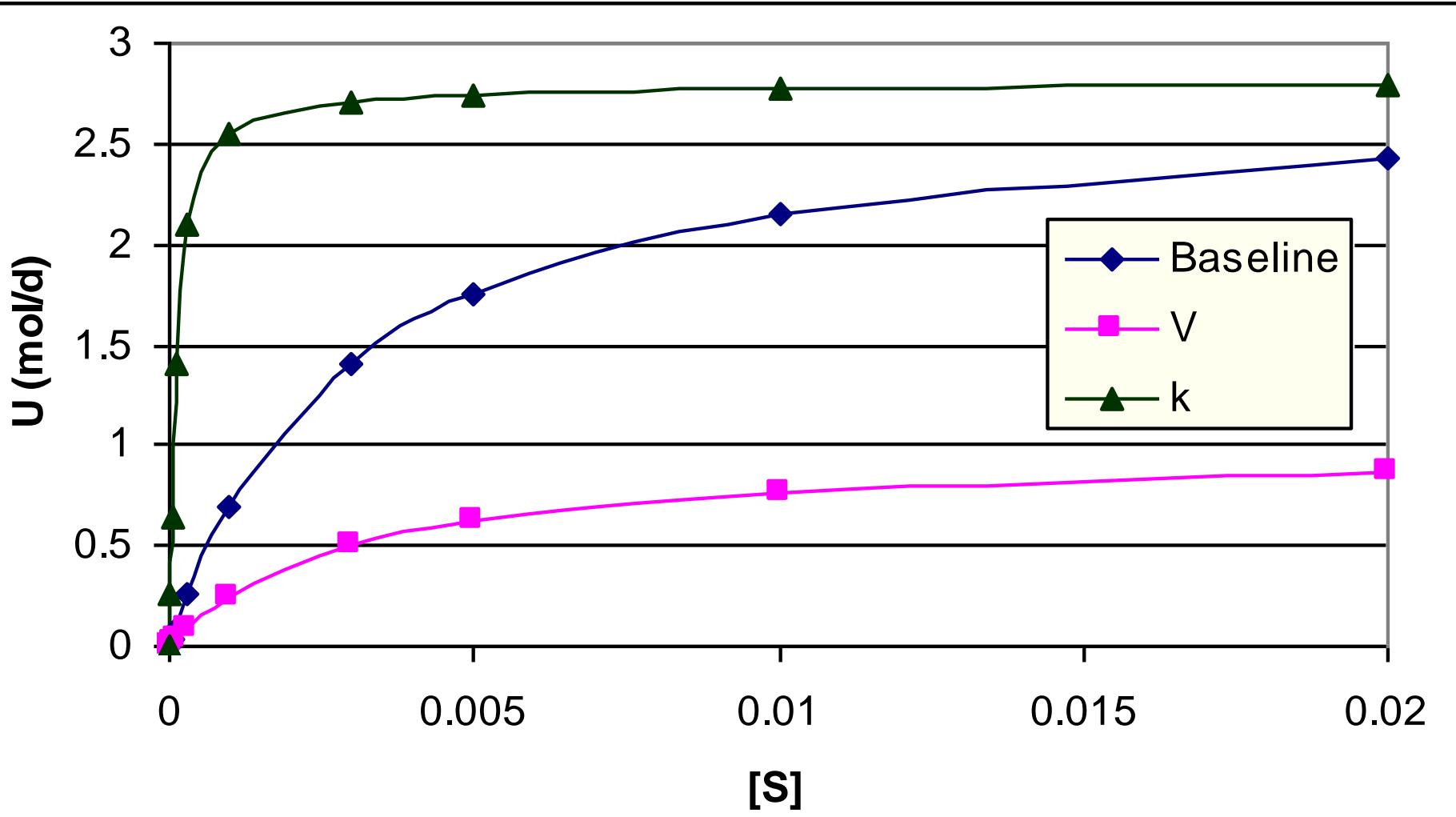
Integrate  $dFa/dt = \text{Mol Fa}$

$$cFa = Fa / \text{Blood volume} \\ = \text{Mol/L}$$

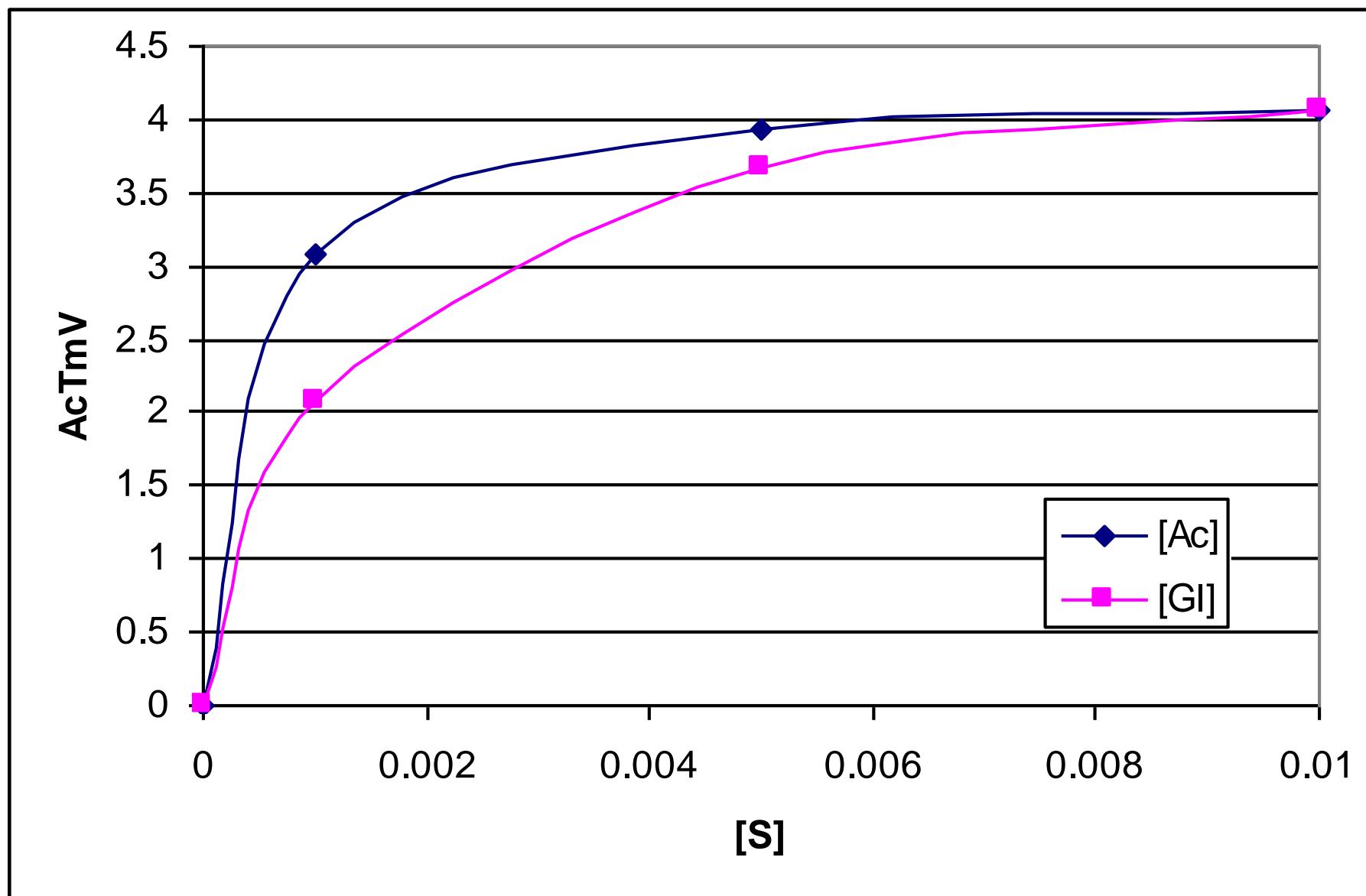
$$\frac{dAc}{dt} = absAc + TAaAc - AcTsF - AcTmV - AcCd$$



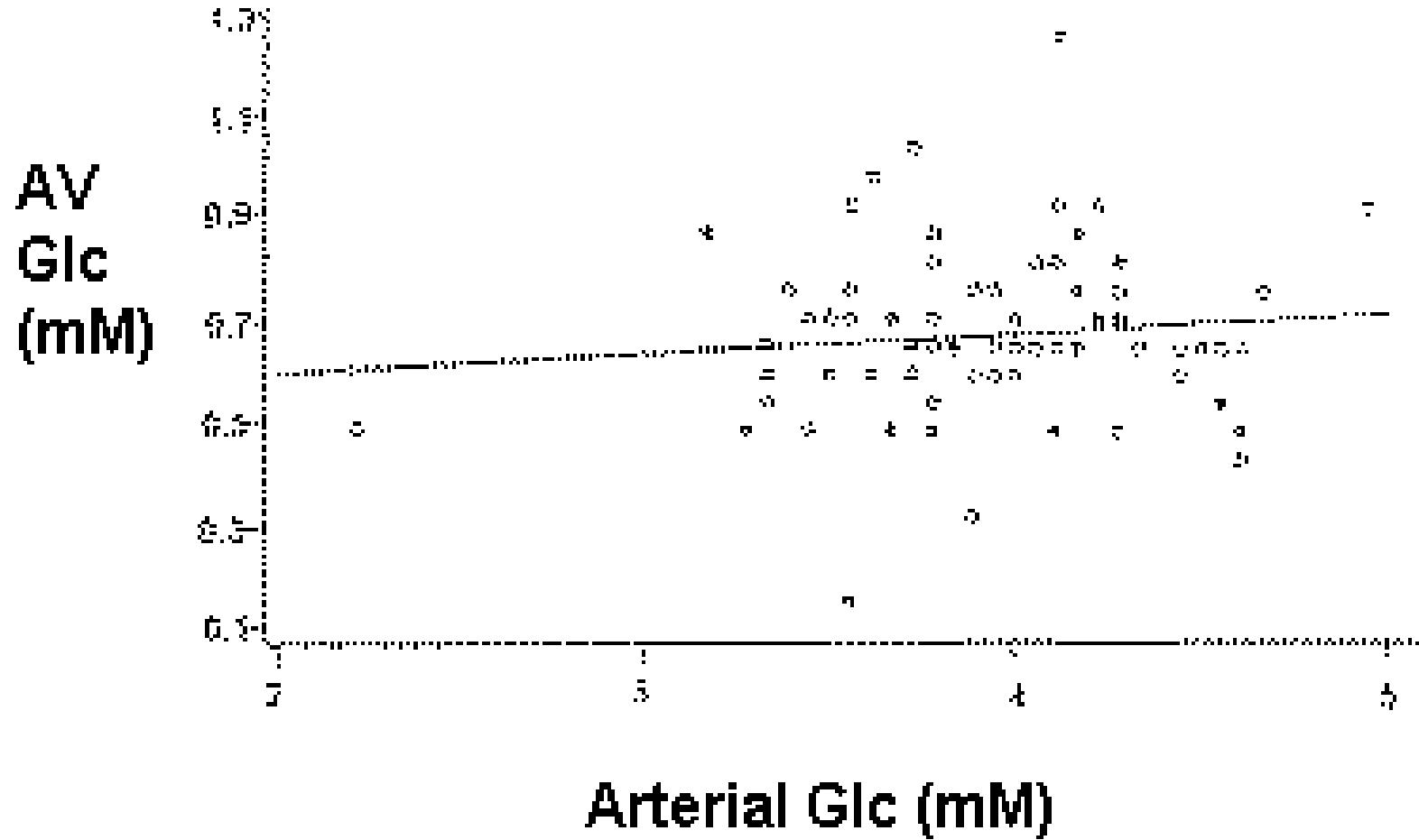
# Example: $U = V_m / (1 + K_m/[S])$



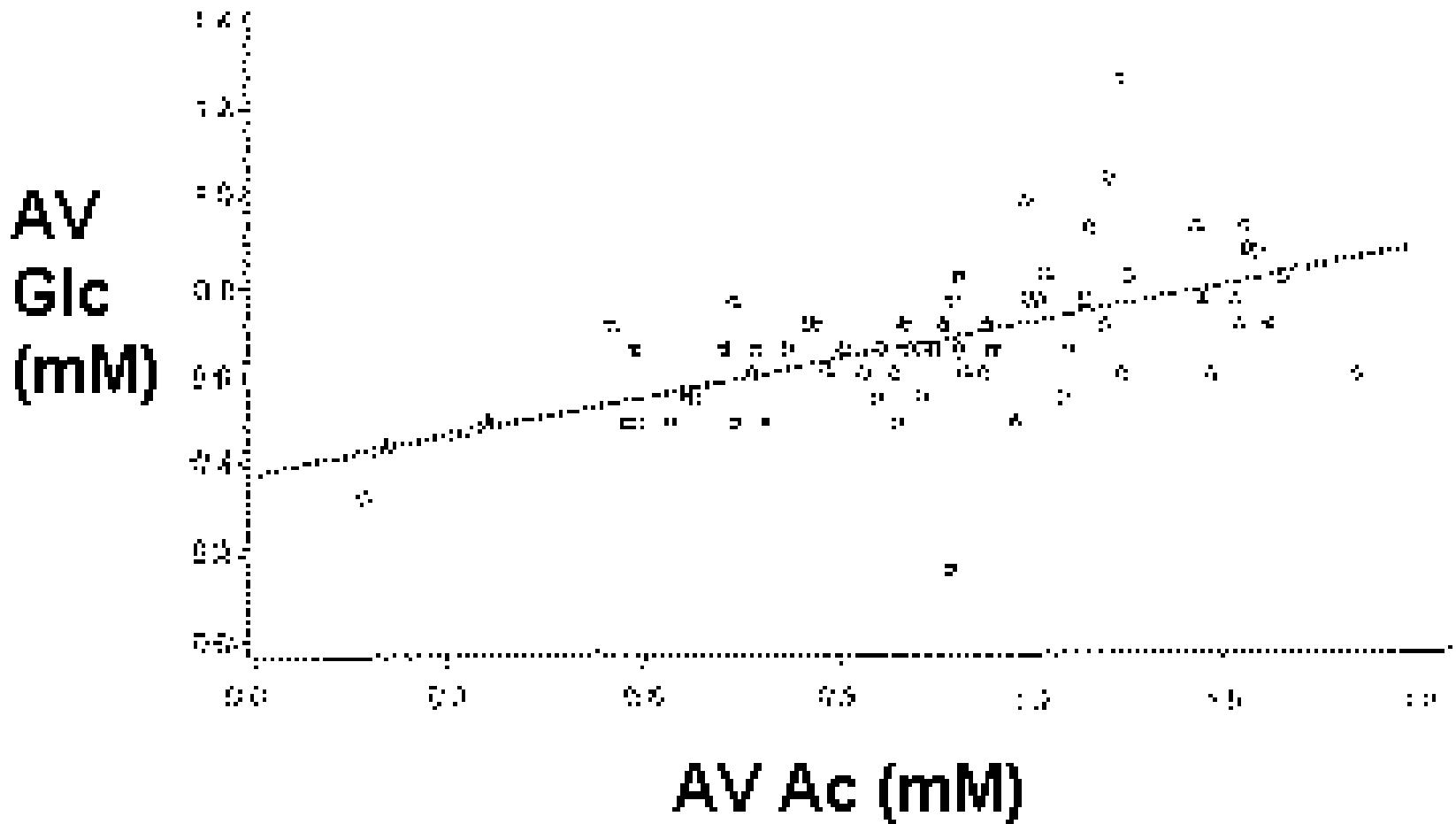
$$\text{AcTmV} = V_{\text{AcTmV}} * uenz * K_{minh} * \text{INS} \\ / (1.0 + k_{\text{AcTmV}} / [\text{Ac}] + k_1 \text{AcTm} / [\text{GI}])$$



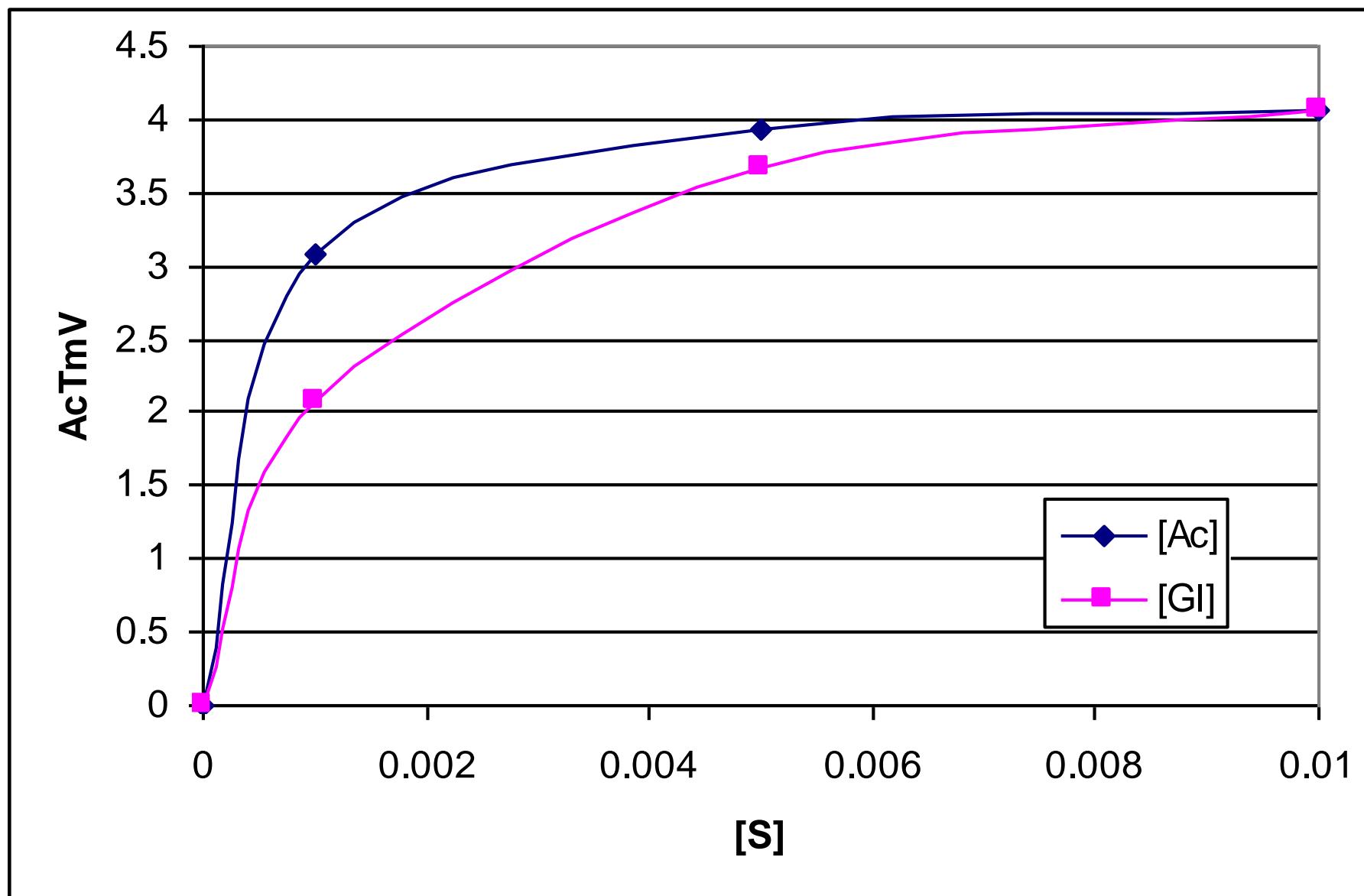
# AV Difference (Mammary)



# AV Difference (Mammary)

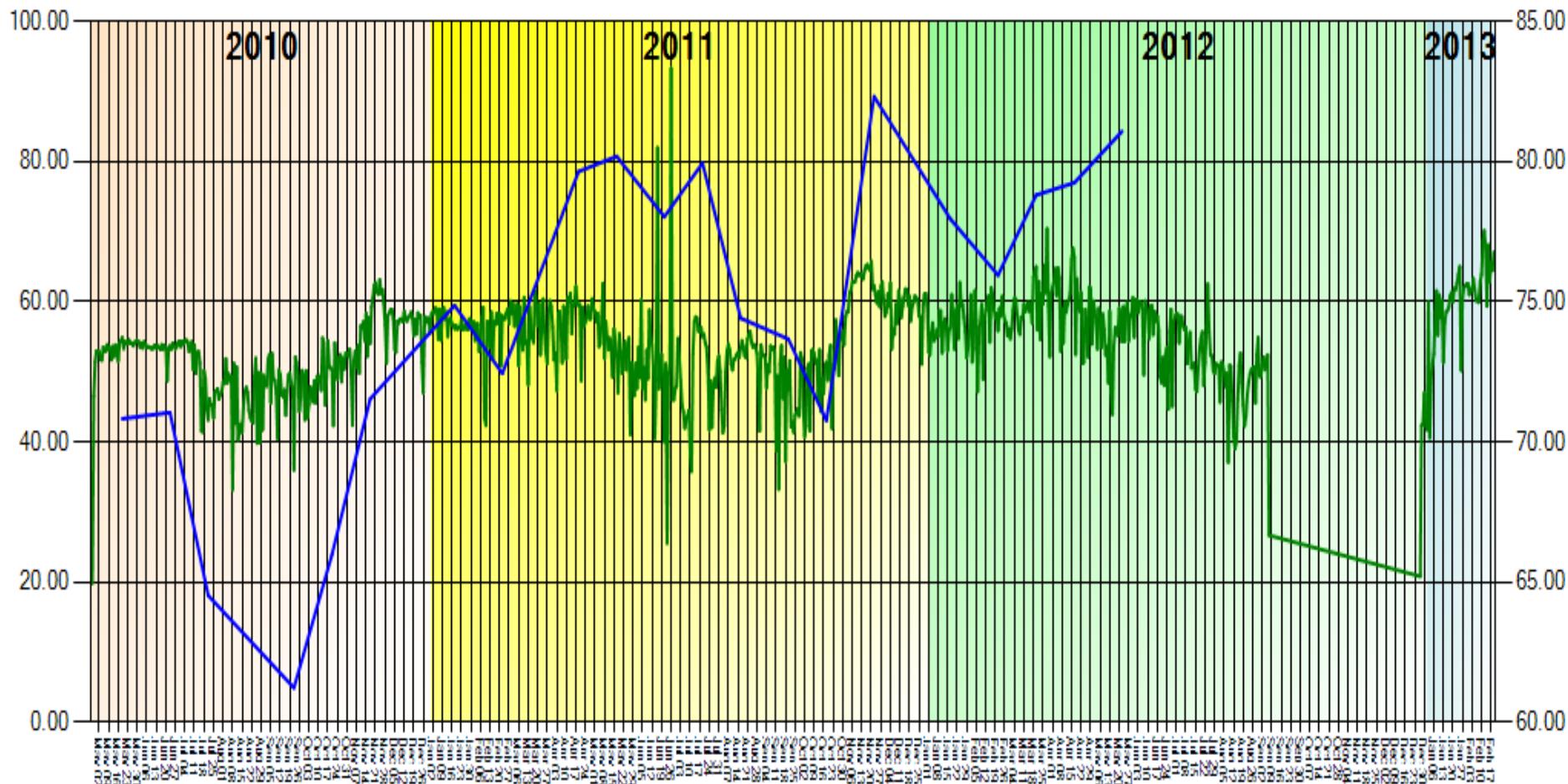


$$\text{AcTmV} = V_{\text{AcTmV}} * uenz * K_{minh} * \text{INS} \\ / (1.0 + k_{\text{AcTmV}} / [\text{Ac}] + k_1 \text{AcTm} / [\text{GI}])$$

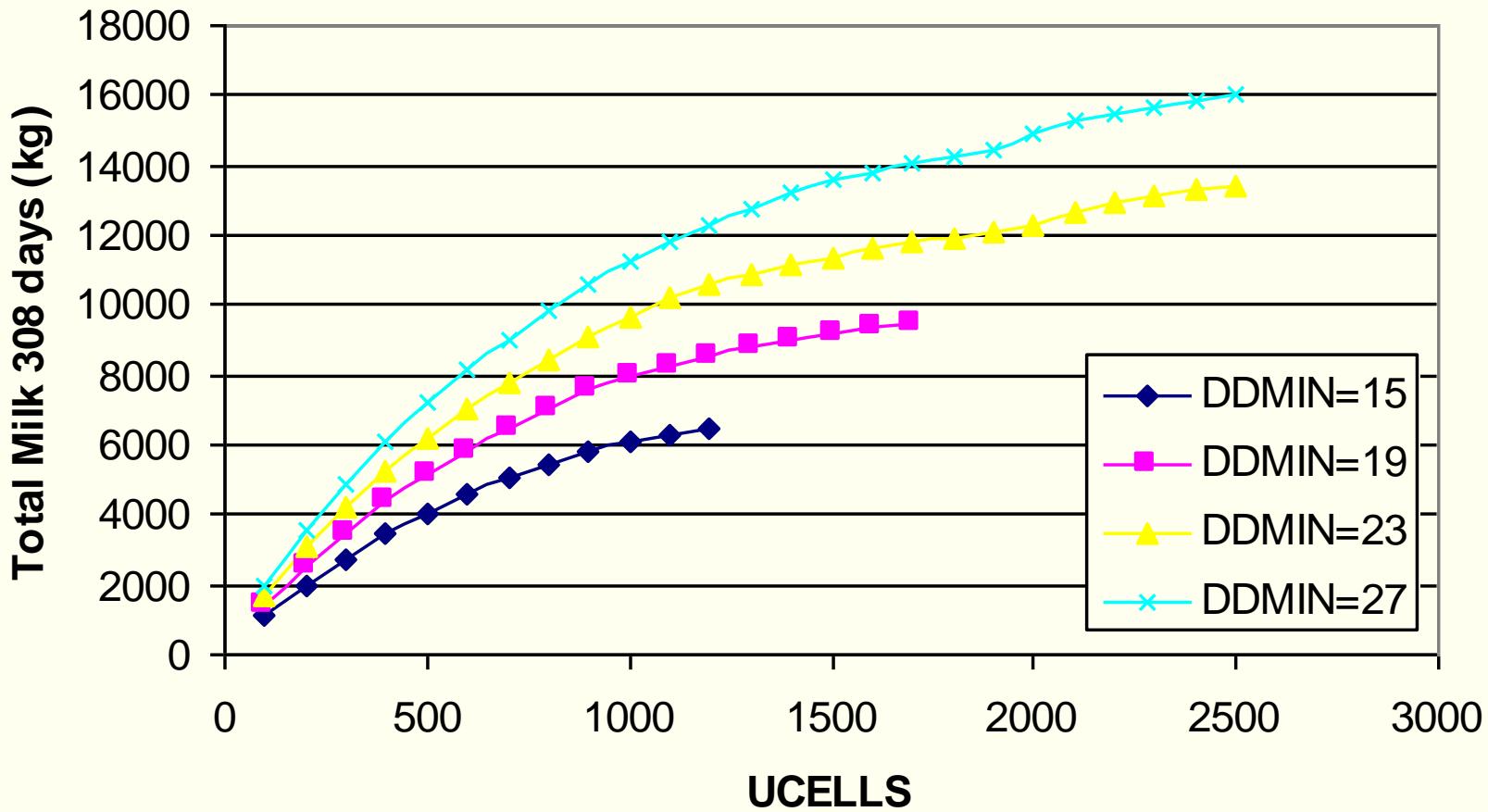


# Representation of milk production

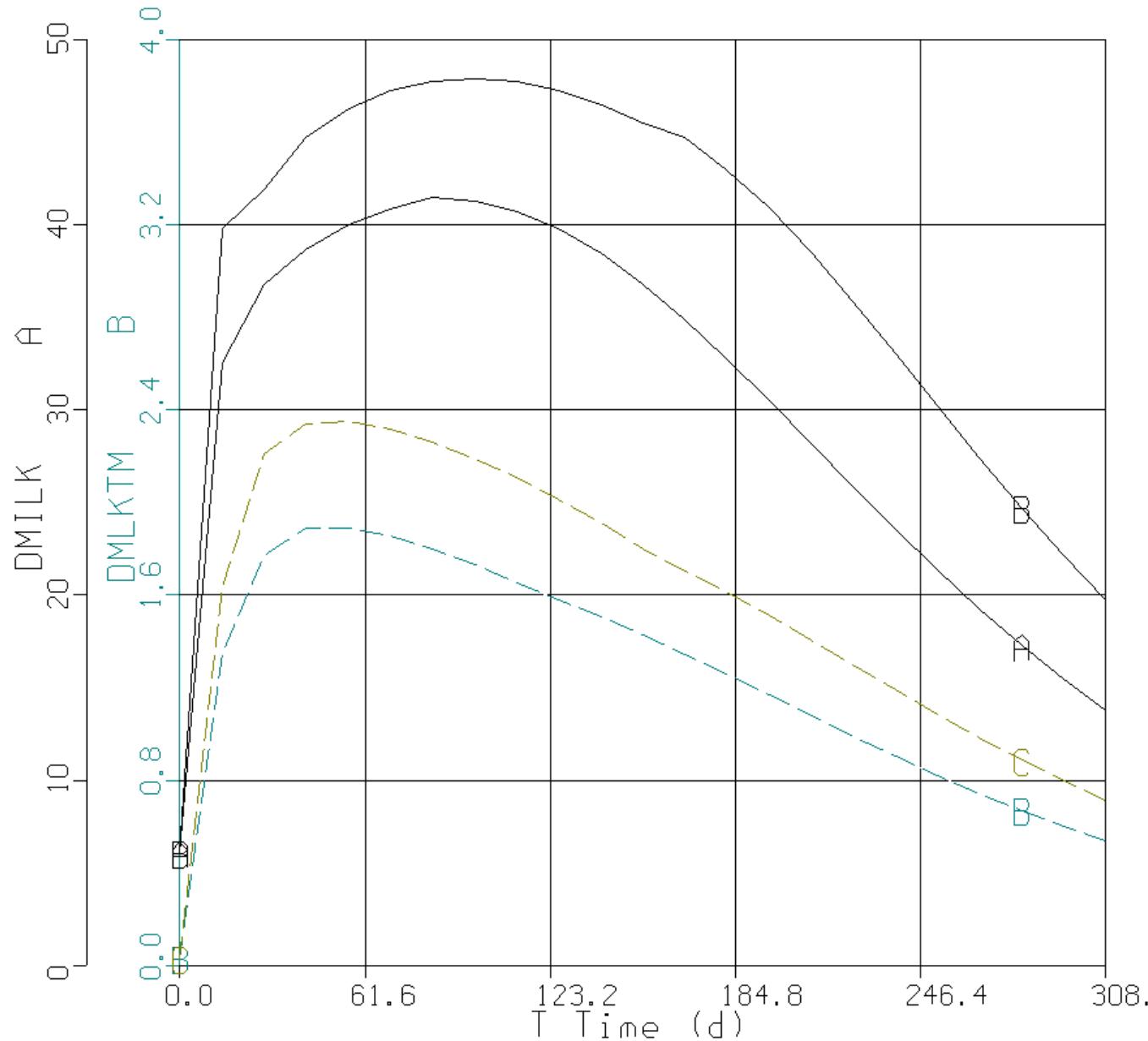
Intake (Actual DMI/hd/day) for Milking\* vs Milk Production (PenMilk lbs/hd/day) for Milking\*



# Molly Milk Production vs. DMI



# Potential milk = UCCELLS



# Molly milk production assumptions

1. Lactose is 4.8% of milk yield
2. Lactose production is dependent on  $\alpha$ -lactalbumin production
3. Relative proportion of milk fat from de novo (Ac) and body, diet (Fa) are 50/50
4. Milk protein yield is determined by limiting amino acid theory.

# Representation of milk production

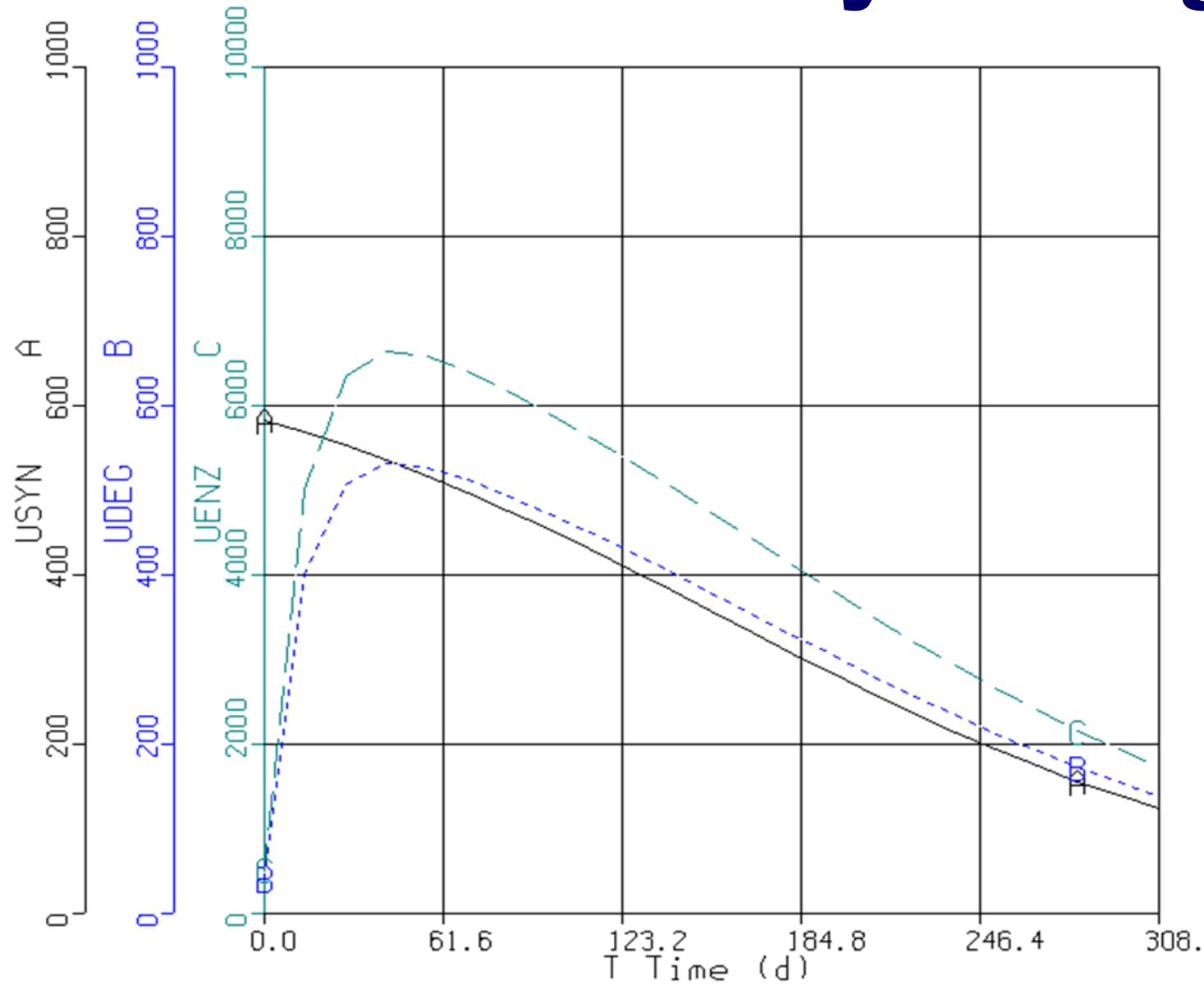
**duenz = usyn - udeg**

**usyn = Vusyn\*UCELLS\*Lhor\*BST/**  
**(kusyn+Lhor\*BST)**

**udeg = uenz\*(Kudeg + KudegM\***  
**((umave/Kmdeg)<sup>10</sup>/(1+umave/Kmdeg)<sup>10</sup>))**

**= retained milk effects**  
**Lhor is integrated**

# **duenz = usyn - udeg**



# Milk Components

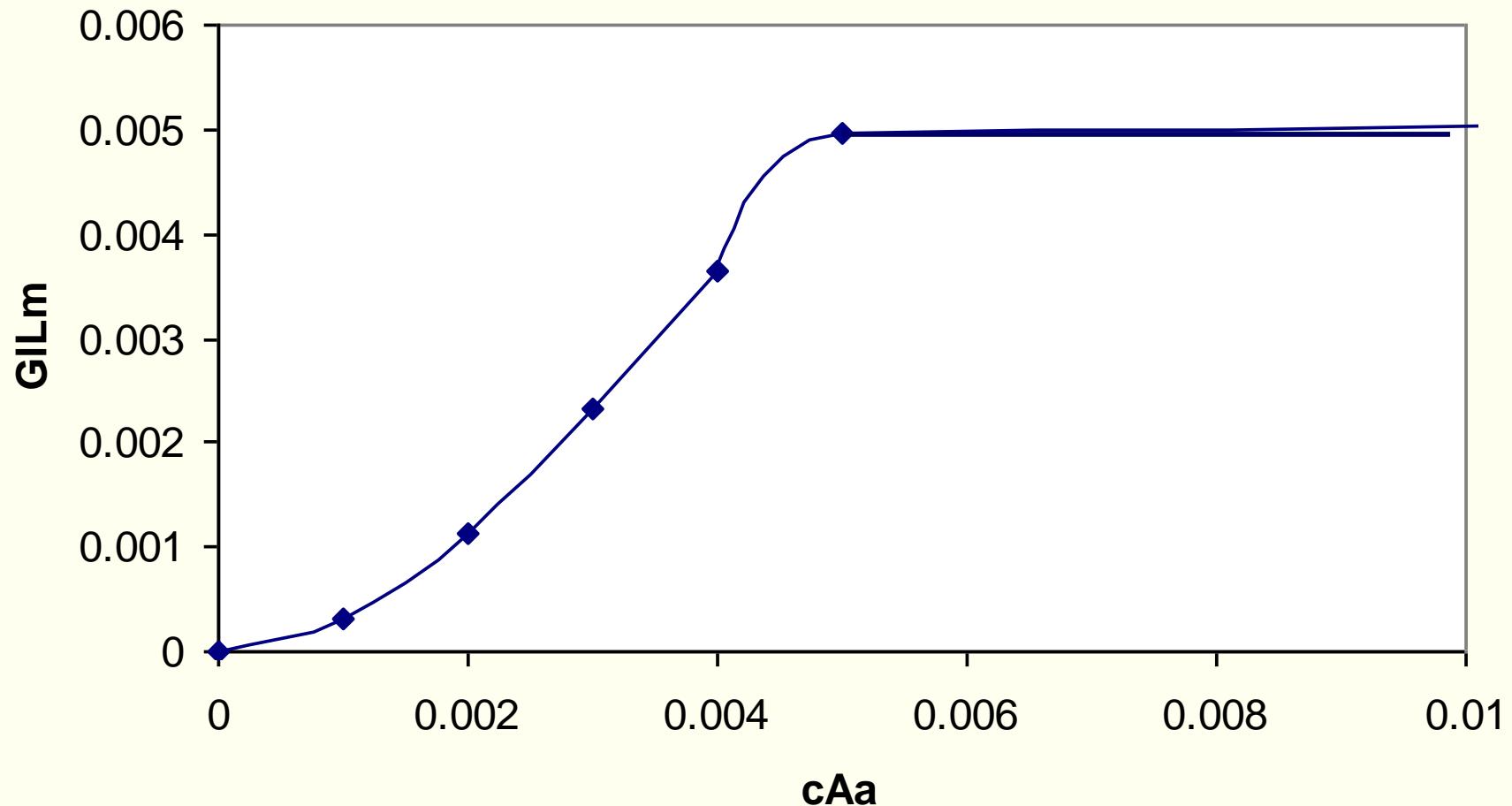
$$1. \text{ GI}_{\text{LmV}} = V_{\text{GI}_{\text{Lmf}}} * (V_{\text{AaLA}} * u_{\text{enz}} * k_{\text{minh}} / (1 + ((k_{\text{AaLA}} / [\text{Aa}])^{\text{EXP}})) / f_{\text{LAAa}}$$

$$2. \text{ Fa}_{\text{TmV}} = V_{\text{Fa}_{\text{TmV}}} * u_{\text{enz}} * I_{\text{NS}} * k_{\text{minh}} / (1 + k_{\text{Fa}_{\text{TmV}}} / [\text{Fa}] + k_{1_{\text{FaTm}}} / [\text{GI}])$$

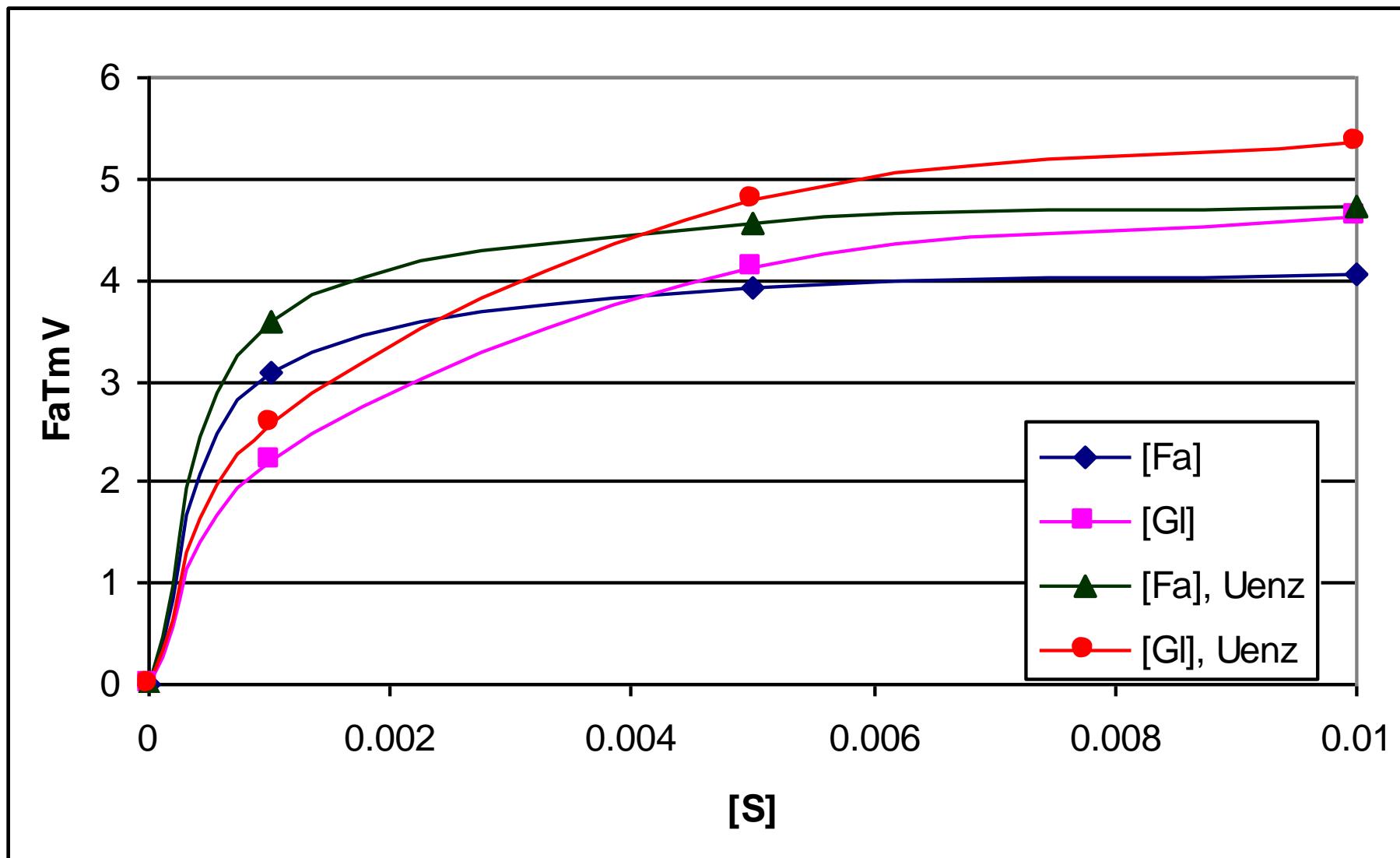
$$3. \text{ Ac}_{\text{TmV}} = V_{\text{Ac}_{\text{TmV}}} * u_{\text{enz}} * I_{\text{NS}} * k_{\text{minh}} / (1 + k_{\text{Ac}_{\text{TmV}}} / [\text{Ac}] + k_{1_{\text{AcTm}}} / [\text{GI}])$$

$$4. \text{ Aa}_{\text{PmV1}} = V_{\text{AaPm}} * u_{\text{enz}} * k_{\text{minh}} / (1 + (k_{\text{AaPm}} / [\text{Aa}])^{\text{EXP}}) / f_{\text{PmAa}}$$

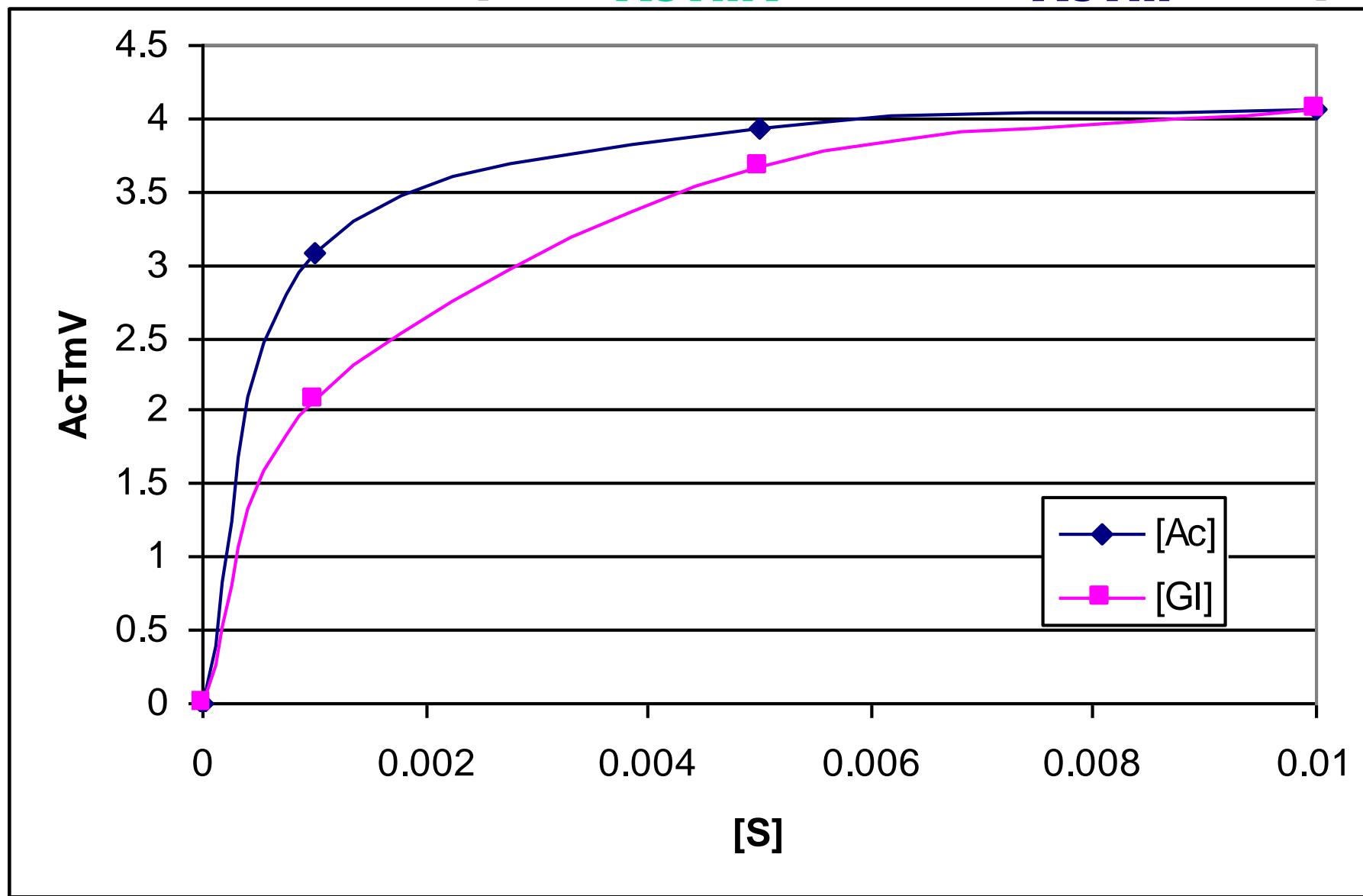
$$GILmV = V_{GILmf} * (V_{AaLA} * uenz * kminh / (1 + ((k_{AaLA} / [Aa])^{\text{EXP}}))) / fLAAa$$



$$FaTmV = V_{FaTmV} * uenz * INS * kminh / \\ (1 + k_{FaTmV}/[Fa] + k1_{FaTm}/[GI])$$



$$\text{AcTmV} = V_{\text{AcTmV}} * uenz * \text{INS} * \text{kminh} / \\ (1 + k_{\text{AcTmV}} / [\text{Ac}] + k_{\text{AcTm}} / [\text{GI}])$$



$$AaPmV1 = V_{AaPm} * uenz * kminh / \\ (1 + (k_{AaPm} / [Aa])^{EXP}) / fPmAa$$

 Limiting Amino Acids			
AaPbB1 27.41742	AaPvV1 15.22529	AaPmV1 20.26647	AaLA1 1.496554
SAaPb1 24.05846	SAaPv1 13.68130	SAaPm1 11.18644	SAaLA1 0.841276
LysPb1 24.00315	LysPv1 12.95303	LysPm1 11.47371	LysLA1 0.844787
HisPb1 35.09698	HisPv1 19.01847	HisPm1 76.13619	HisLA1 6.579670



## Input Simulation Data

## Initial Simulation Settings

Initial Bodyweight 700

Udder Cells 1000

 Body Fat % 0.207 BCS (1-5) 3.2

Length of Simulation Long

Milk Price \$/kg

Go Until day 70

Milking Continuous

Conception at Day 90

Select a Diet List

Standard Diet List

Select Diet diet1

## Intake 1

Fixed Intake (kg/d)

Fixed Intake 11

## Intake 2

Intake based on Milk

Intake (kg) / kg milk 0.33

BST at 1.0 times basal

Ionophore 

Diet Price \$/kg

## Abomasum Infusions (moles AA/d or kg Protein/d)

Sulfur AA 0

Lysine 0

Histidine 0

Casein 0

Enter ACSL CMD

Log variables over time Save data for multiple lactation plots 

## Milk Production

 KG LB

Time (d) 70

Daily milk yield kg 40.81751

Total milk kg 2446.653

Total milk lactose kg 117.4393

Total milk protein kg 75.38944

Total milk fat kg 112.8343

## Acetate

Time (d)  
70

absAc

69.08464

cAc

78.0172424316406

TAaAc

3.593405

AcCd

33.59507

AcTsF

10.67335

AcTmV

28.18128

## Fatty Acids

Time (d)  
70

absFa

2.636204

cFa

3.54315304756165

TsFaF1

5.90887619182467E-04

FaCd

1.655520

FaTsF

6.354977

FaTmV

3.380170

## General Production

 KG LB

Time (d) 70

kg BW

728.9989

kg EBW

599.6323

BCS

2.0423316

DMI kg/d

24.31850

Tot DMI kg

1535.231

Profit /d

6.4283118

kg Lean Body

417.5971

Feed Cost /

4.4536280

kg viscera

90.78244

Profit /Sim

390.40472

kg adipose

91.25265

## Glucose

Time (d) 70

PrCdV 10.34290

absPr

34.47634

PrGIV1

12.06672

TAaGI

3.130599

LaGIV1

15.04781

GyGIV1

2.021699

absGI

11.42089

UpGI

1.142089

GILmV 11.46350

GIHyF 1.869971

GITpF 2.582765

GILaB 4.028314

GIHyV 4.937362

GITpV 0.646374

GICd 7.877070

GGIla

20.55761

## Limiting Amino Acids

AaPbB1

27.545820

AaPvV1

15.153165

AaPmV1

20.233058

AaLA1

1.4940869

SAaPb1

24.163116

SAaPv1

13.626000

SAaPm1

11.166792

SAaLA1

0.8397984

LysPb1

24.008815

LysPv1

12.847830

LysPm1

11.257755

LysLA1

0.8288865

HisPb1

35.105587

HisPv1

18.864179

HisPm1

71.202682

HisLA1

6.1533174

# Demo using BST

## 1. Control

Go until day 308

Diet1

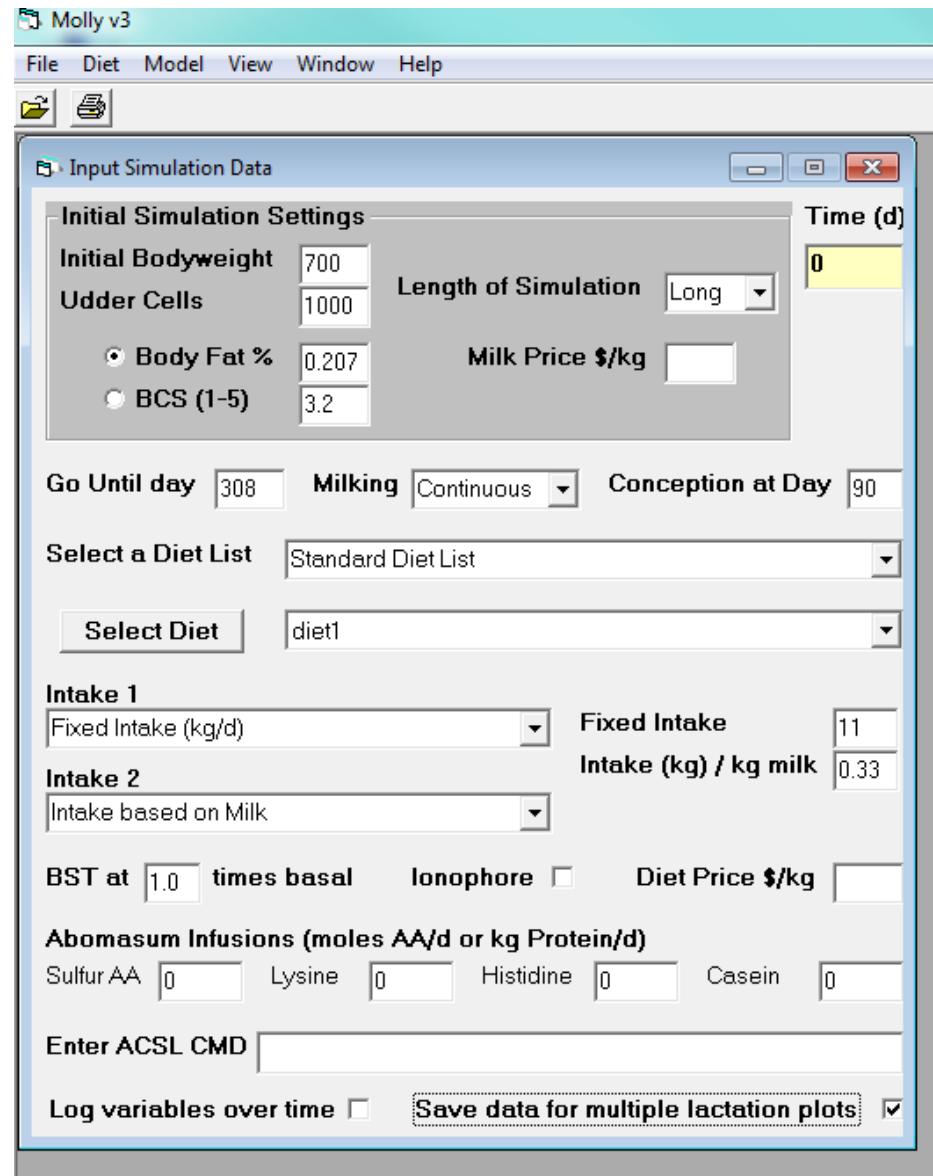
BST 1.0

Save data....

Model load

Model reset to T=0

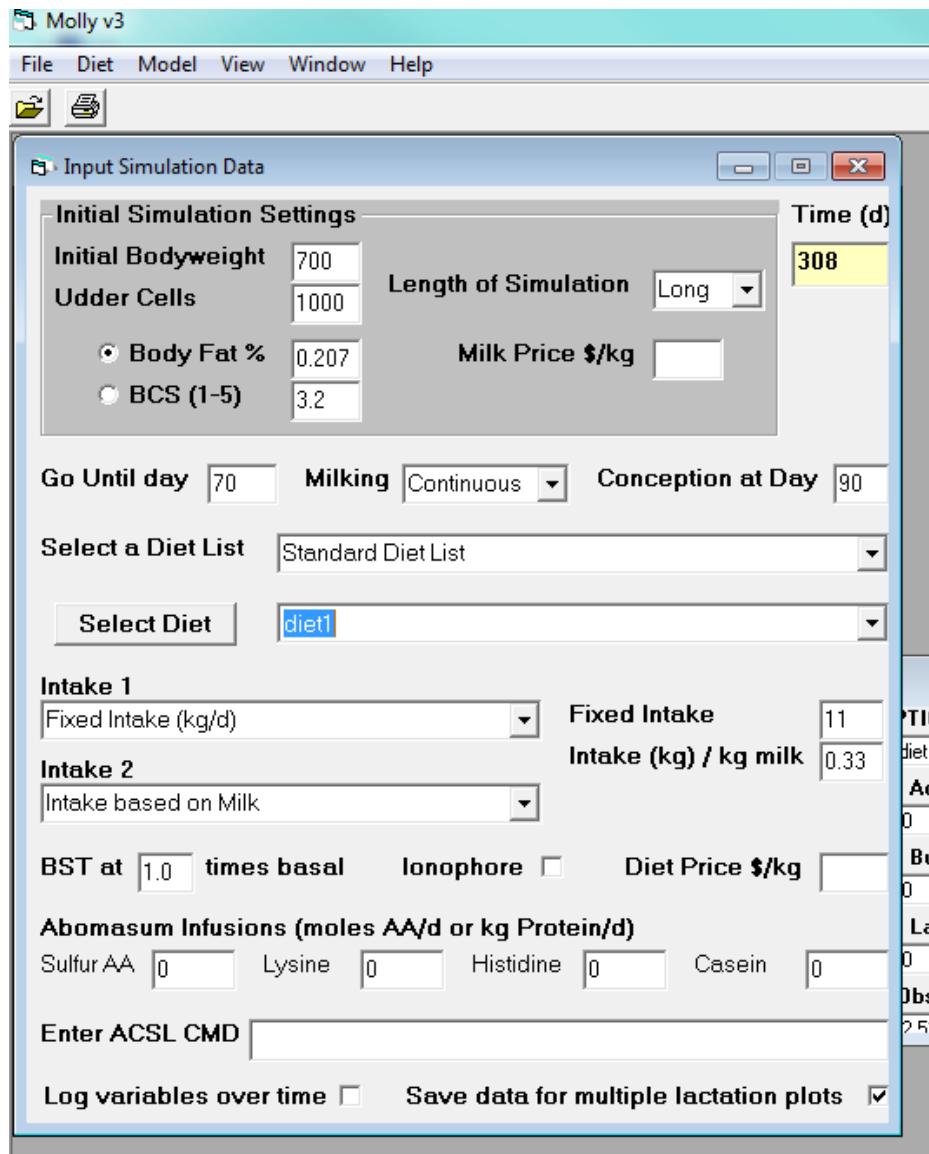
Model run



# Demo using BST

2. BST lactation  
Go until day 70  
Diet1  
BST 1.0  
Save data....

Model reset to T=0  
Model run

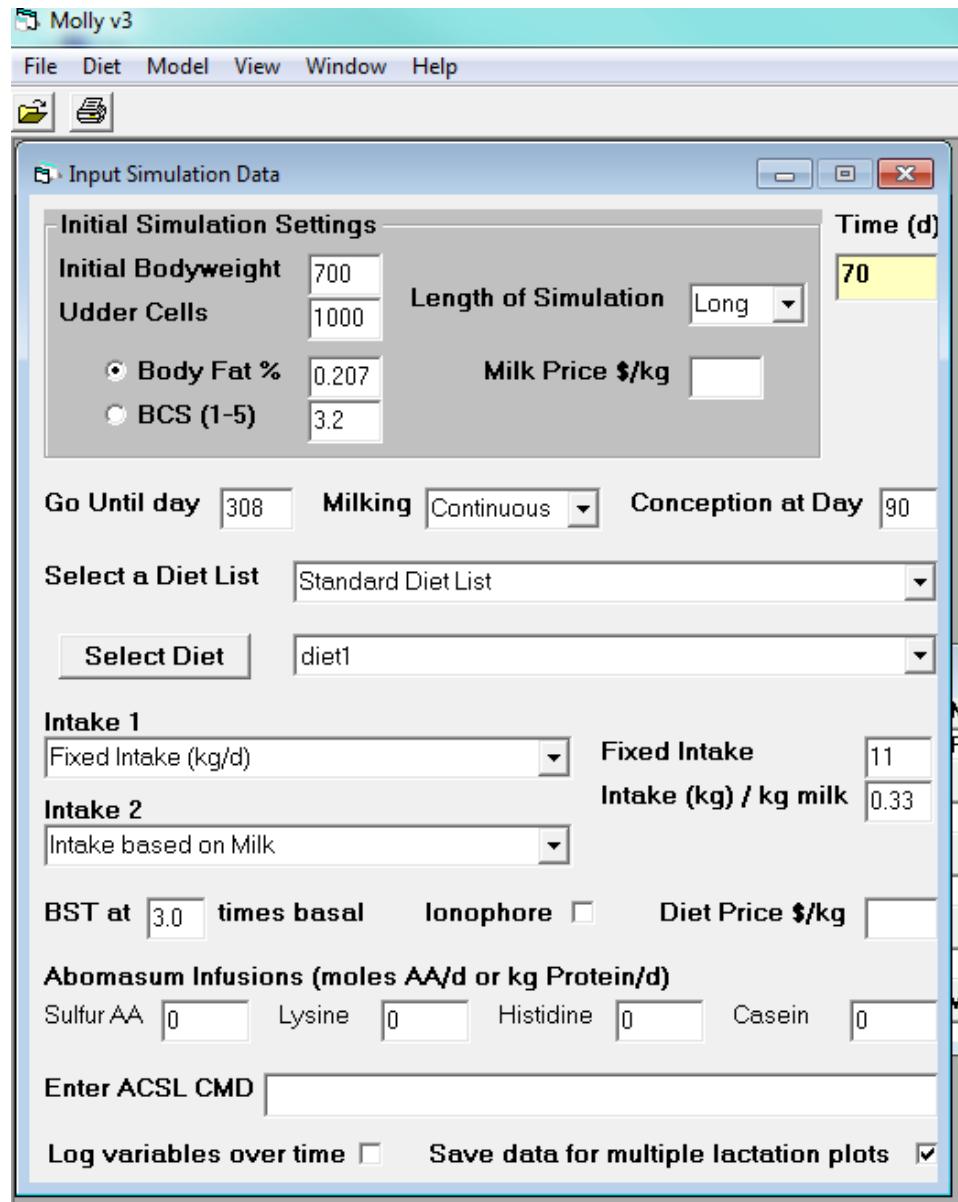


# Demo using BST

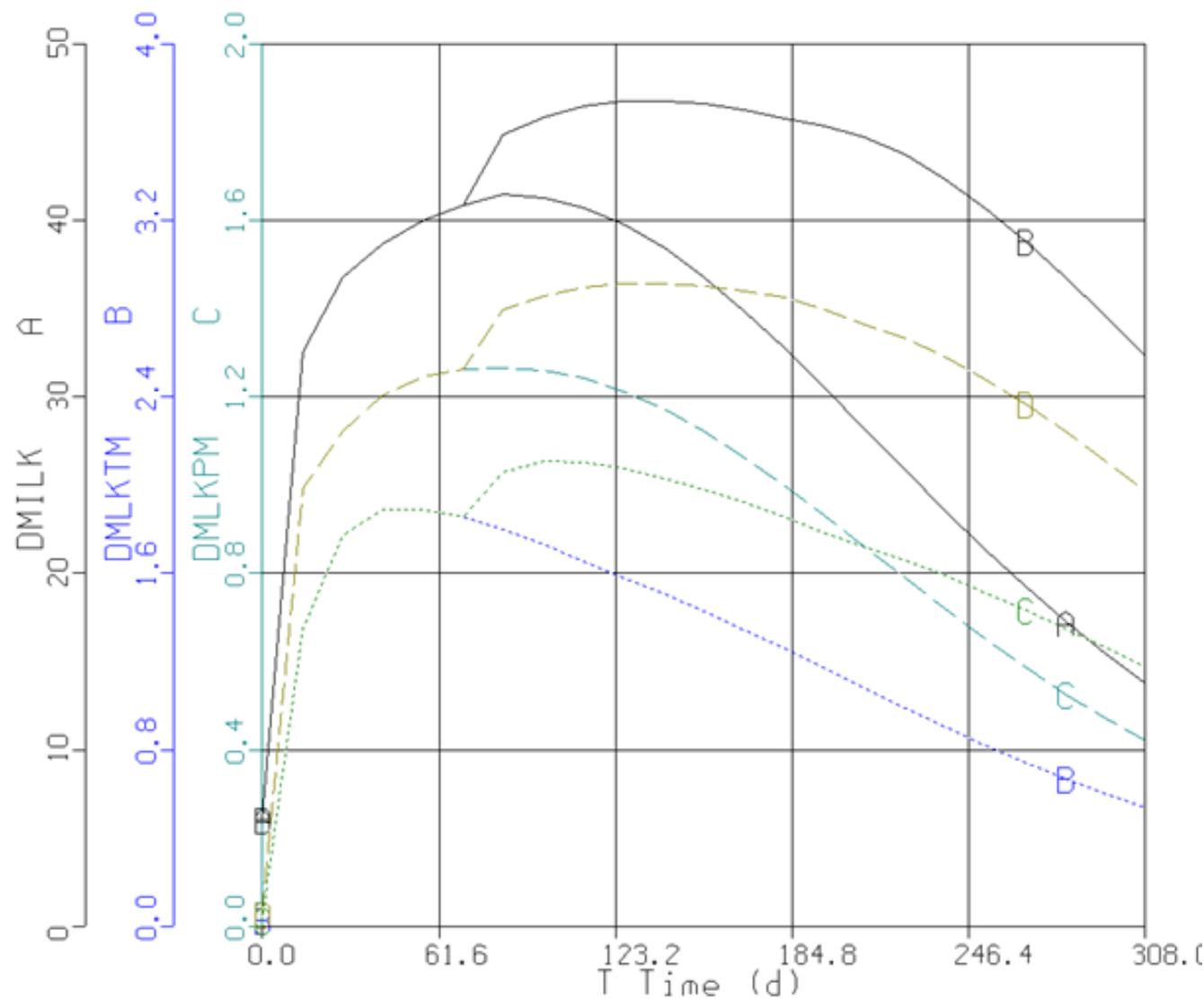
3. Give BST  
Go until day 308  
Diet1  
BST 3.0  
Save data....

Model Continue

View Plot  
Dmilk  
Dmlktm  
dmlkpm



# Results

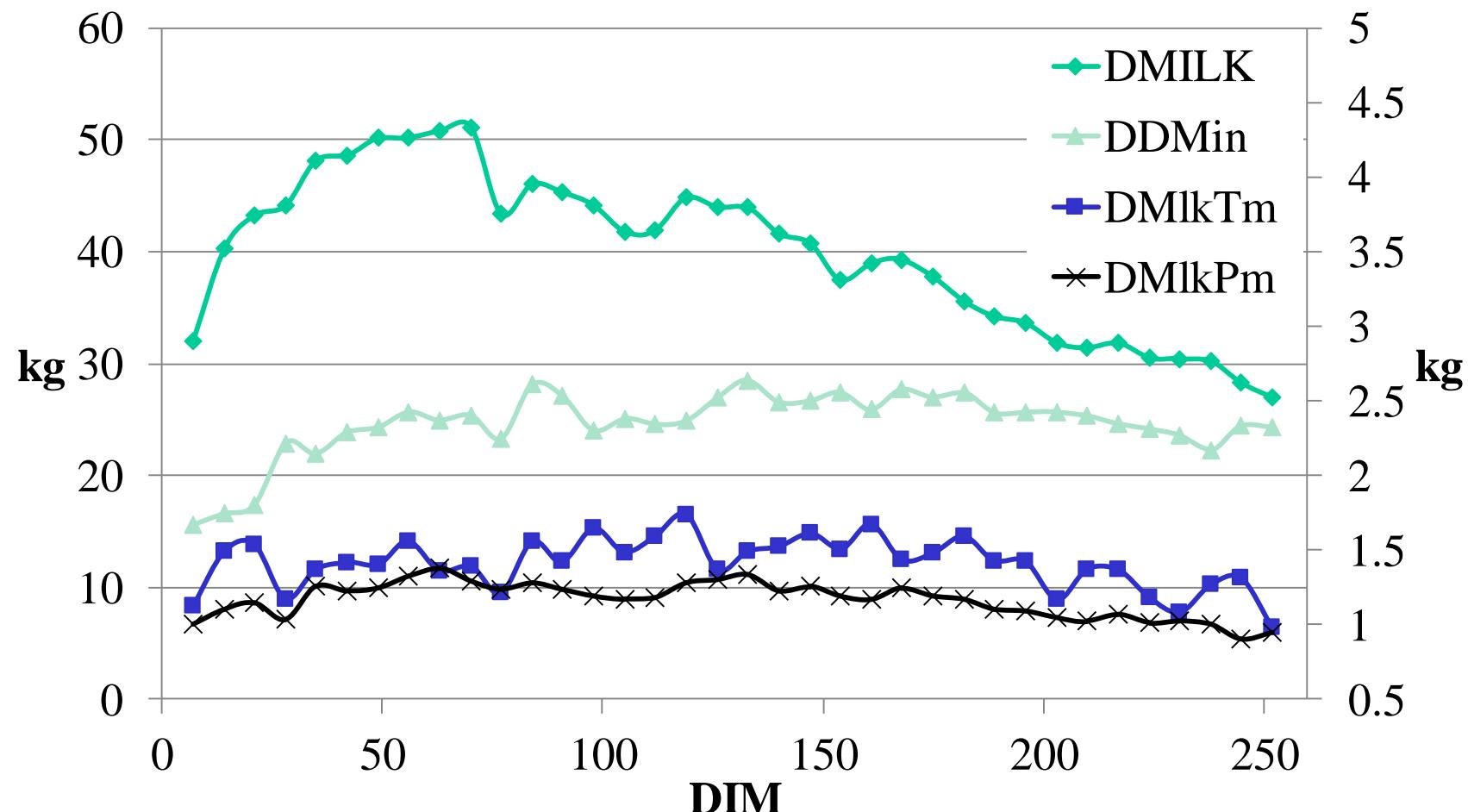


# Modeling Exercise

Adjust ucells to match the cow's milk production

Total milk = 10042, total fat=355, total protein=293

iBW = 550, fBW=612, tot DMI=6197



# Modeling Exercise

Molly v3

File Diet Model View Window Help

**Input Simulation Data**

**Initial Simulation Settings**

- Initial Bodyweight: 550
- Udder Cells: 1000
- Length of Simulation: Long (Time: 0)
- Body Fat %: 0.207
- BCS (1-5): 3.2
- Milk Price \$/kg: [empty]
- Go Until day: 252
- Milking: Continuous
- Conception at Day: 90
- Select a Diet List: Standard Diet List
- Select Diet: diet1
- Intake 1**: Fixed Intake (kg/d) 11, Intake (kg) / kg milk 0.33
- Intake 2**: Intake based on Milk
- BST at 1.0 times basal, Ionophore:
- Diet Price \$/kg: [empty]
- Abomasum Infusions (moles AA/d or kg Protein/d)
- Sulfur AA: 0, Lysine: 0, Histidine: 0, Casein: 0
- Enter ACSL CMD: s vactmv=0.012, vfatmv=0.0014
- Log variables over time:
- Save data for multiple lactation plots:

**Milk Production**

- Time (d): 0
- Daily milk yield kg: 5.555499
- Total milk kg: 5.555499
- Total milk lactose kg: 0
- Total milk protein kg: 0
- Total milk fat kg: 0
- Milk Protein %: 5.555499
- Milk Lactose %: 5.555499
- Milk Fat %: 5.555499

**General Production**

- Time (d): 0
- BCS: 5.5554998
- kg BW: 5.555499
- kg EBW: 5.555499
- DMI kg/d: 5.555499
- Tot DMI kg: 0
- Feed Cost /d: 5.5554998
- kg Lean Body: 5.555499
- kg viscera: 5.555499
- kg adipose: 5.555499
- Profit /d: 5.5554998
- Profit /Sim: 0

**User Defined Variables**

MOLLY Model Variables:

	Time(d)
ABSLRA	1.39999995008111E-03
ABSRPR	5.55549980048088E+33
ABSSAA	5.55549980048088E+33
ACACTS	1.40000004321337E-02
ACCD	5.55549980048088E+33
ACCDAT	5.55549980048088E+33
ACCDCC	5.55549980048088E+33
ACCDEG	5.55549980048088E+33
ACCDGF	5.55549980048088E+33
ACCOR	5.55549980048088E+33
ACCPRTIN	5.55549980048088E+33
ACFAAAD	5.55549980048088E+33
ACTGTG	5.55549980048088E+33
ACTMH1	5.55549980048088E+33
ACTMH2	5.55549980048088E+33
ACTMH3	5.55549980048088E+33
ACTMV1	5.55549980048088E+33
ACTMV	5.55549980048088E+33
ACTSF1	5.55549980048088E+33
ACTSF	5.55549980048088E+33
ACTSH1	5.55549980048088E+33

**Create Plot**

X AXIS

- X Variable Name: T
- X Axis Label: Time (d)
- X Axis Range: Low: 0, High: 0

Y AXIS

- Y Variable: dmilk
- Style: Solid
- Width: 1
- Low: [empty], High: [empty]

- Y Variable: dmin
- Style: Dash
- Width: 1
- Low: [empty], High: [empty]

- Y Variable: dmlktm
- Style: Dot
- Width: 1
- Low: [empty], High: [empty]

- Y Variable: dmilkpm
- Style: Solid
- Width: 1
- Low: [empty], High: [empty]

- Y Variable: [empty]
- Style: Dash
- Width: 1
- Low: [empty], High: [empty]

- Y Variable: [empty]
- Style: Dot
- Width: 1
- Low: [empty], High: [empty]

PLOT

CANCEL

# Modeling Exercise - Solution

Molly v3

File Diet Model View Window Help

**Input Simulation Data**

**Initial Simulation Settings**

- Initial Bodyweight: 550
- Udder Cells: 1064
- Length of Simulation: Long (Time: 252)
- Body Fat %: 0.207
- BCS (1-5): 3.2
- Milk Price \$/kg: [empty]

Go Until day: 252 Milking: Continuous Conception at Day: 90

Select a Diet List: Standard Diet List

Select Diet: diet1

**Intake 1**

- Fixed Intake (kg/d): 11.4
- Intake (kg) / kg milk: 0.33

**Intake 2**

- Intake based on Milk

BST at: 1.0 times basal Ionophore:  Diet Price \$/kg: [empty]

**Abomasum Infusions (moles AA/d or kg Protein/d)**

- Sulfur AA: 0 Lysine: 0 Histidine: 0 Casein: 0

Enter ACSL CMD: s vactmv=0.0111, vfatmv=0.0013

Log variables over time:  Save data for multiple lactation plots:

**Milk Production**

- Time (d): 252
- Daily milk yield kg: 24.09516
- Milk Protein %: 3.049683
- Total milk kg: 10047.15
- Milk Lactose %: 4.799999
- Total milk lactose kg: 482.2634
- Milk Fat %: 3.301534
- Total milk protein kg: 309.2997
- Total milk fat kg: 354.8433

**General Production**

- Time (d): 252
- BCS: 5.0718245
- kg BW: 755.7580 kg EBW: 646.4342
- DMI kg/d: 20.24779 Tot DMI kg: 6197.983
- kg Lean Body: 338.6249
- kg viscera: 75.38240
- kg adipose: 232.4270
- Feed Cost /d: 3.1800630
- Profit /d: 3.1711533
- Profit /Sim: 1694.0550

**User Defined Variables**

MOLLY Model Variables:	Time(d)
VAAPVV	0.454591453075409
VAC	
<b>VACTMV</b>	<b>10.9101076126099</b>
VACTSCOR	
VACTSDEG	
VACTSF	
VACTSSYN	
VCSFV	
VDNAMX	
VDNAPR	
VFA	
VFAEFF	
VFATMV	0.529828190803528
VFATSF	
VGL	
VGLLAB	
VGLLMF	
VGLTPF	
VGLTPV	
VHISDEG	
VHISLA	

**Create Plot**

X AXIS

- X Variable Name: T
- X Axis Label: Time (d)
- X Axis Range: Low: 0 High: 252

Y AXIS

- Y Variable: dmilk
- Style: Solid
- Width: 1
- Low: [empty] High: [empty]

- Y Variable: ddmmin
- Style: Dash
- Width: 1
- Low: [empty] High: [empty]

- Y Variable: dmilktn
- Style: Dot
- Width: 1
- Low: [empty] High: [empty]

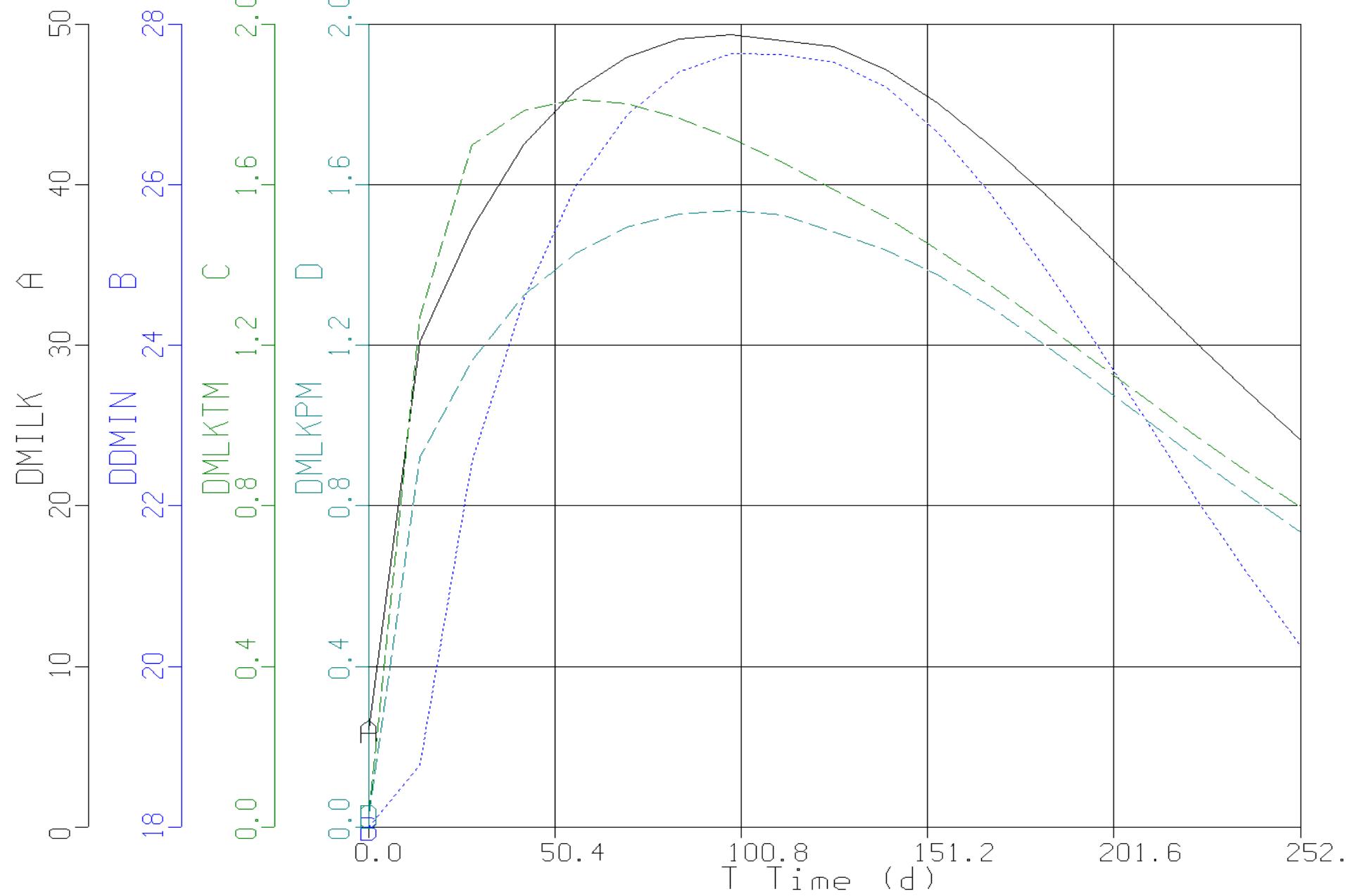
- Y Variable: dmilkpm
- Style: Solid
- Width: 1
- Low: [empty] High: [empty]

- Y Variable: [empty]
- Style: Dash
- Width: 1
- Low: [empty] High: [empty]

- Y Variable: [empty]
- Style: Dot
- Width: 1
- Low: [empty] High: [empty]

PLOT CANCEL

# Modeling Exercise - Solution



# Thanks...



National Animal Nutrition Program  
Leveraging Resources, Linking Researchers

<http://www.vmtrc.ucdavis.edu/laboratories/metabolic/molly.cfm>